Calculator Programs For Chemical Engineers

Volume II

Edited by the Staff of Chemical Engineering

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Preface

Chemical Engineering is proud to present this second volume of calculator programs for chemical engineers. As in the first volume, all of the programs in this book can be run on the Texas Instruments TI-59 and the Hewlett-Packard HP-67 and HP-97, and quite a few can be handled by the Texas Instruments TI-58. (As well, all the Hewlett-Packard programs can be run on the HP-41C machines.)

The programs included in the two volumes of *Calculator Programs for Chemical Engineers* have all been published in *Chemical Engineering*—but are offered here, and in the first volume, not only in the original calculator language as listed in the magazine article, but with a translation, so that both HP and TI versions are available.

The purpose of the two-book series is to present a library of programmable calculator programs specifically designed to solve chemical engineering problems. Most of the programs offered are design oriented—such as those for sizing control valves, rating heat exchangers, and designing multistage evaporators—while others are included for use in solving such everyday operation tasks as determining flame temperature or optimizing reactor agitation.

The thirty-four programs contained herein run the gamut of useful applications of chemical engineering principles, from engineering mathematics, physical-properties correlations, and engineering economics to fluid flow, and heat and mass transfer. And an introductory article presents a listing of published calculator programs (from all sources, not just from *Chemical Engineering*) of interest to chemical engineers.

Section I
Introduction

Published calculator programs for chemical engineers

Published calculator programs for chemical engineers

Here is a bibliography of programmable-calculator programs of interest to ChEs, that are available in the literature. And, many of the Chemical Engineering programs that are listed here have been translated, so that both HP and TI versions are now available. These program listings appear in either this book or the first volume of *Calculator Programs for Chemical Engineers.* The footnotes following the "Calculator" listing below indicate this information.

John R. Garrett, *Cost Associates International**

☐ Programs for hand-held programmable calculators are an extremely valuable asset to an engineer who needs to produce a result or solution in a short period of time, or who has to solve the same basic problem many times.

However, the time required to develop and debug any program always requires more time than is needed for a manual solution, because results of any new program must be verified by checking against a manually derived result.

Engineers are already aware of the increased productivity that is made possible by the calculator; many subscribe to a users' library of programs, sponsored by a hardware vendor or a programming club. The following bibliographic listing does not replace these libraries, but is intended to serve as an additional source to help the engineer determine if someone has already produced a program that could be useful to him or her.

The following listing is divided into two main categories—one for advanced calculators such as the HP-67/97 and the TI-58/59, and the second for calculators having less capability or flexibility. Within these two main categories, I have attempted to classify programs according to general areas of interest. This is very difficult to do in many cases, and the reader must be aware that some programs are applicable in more than one category.

In the listing, the title of the article is given first, and the author second (reversing the usual bibliographic-citation form). In some cases, the title has been expanded to include program subject matter, as a further guide to the user. The citation also lists the particular programmable calculator to which the program listing is applicable.

The engineer who is doing a literature search will find many titles that sound as though they contain program listings, but which actually contain an abstract or a computational method. Consequently, all of the following listings have been personally verified by me as containing actual calculator programs (except for a small number labeled "narrative").

I hope that by using this list, other engineers and technical personnel can eliminate a great deal of research time, and increase their personal knowledge and individual productivity.

As an aside, in addition to the principal use of this list, many main-frame and minicomputer programmers could easily translate the program algorithms into subroutines for a larger software package.

*At the time of writing this article, the author was a Senior Cost Engineer for Diamond Shamrock Corp.

Programs for principal engineering calculators

Petroleum refining

Title	Author	Calculator	Reference
Solving Engineering Problems on Programmable Pocket Calculators: Stripping and Flashing, 1. Binary Distillation 2. Multicomponent Flash	Robert F. Benenati	HP-67/97[c]	*Chem. Eng.,* Vol. 84, Mar. 14, 1977, pp. 129–132. (See Piping for Part 1)
Streamline Flash Computations with a Calculator Program	Sohrab Mansouri	HP-67/97[a]	*Chem. Eng.,* Vol. 86, Aug. 27, 1979, pp. 99–101
Flash Vaporization Computations for Plant Operations Eased	R. Franklin Parker and I. Harvey Oliver	HP-67/97	*Oil & Gas J.,* Vol. 77, Dec. 17, 1979, pp. 76–79
How Steam Alters V-L of Crude	T. A. Abdel-Halim	TI-58/59	*Hydrocarbon Process.,* Vol. 59, Jan. 1980, pp. 115–119
Hand Calculator Program Speeds Flash Calculations	I. Harvey Oliver	HP-67/97/ 41C	*Oil Gas J.,* Vol. 78, Mar. 31, 1980, pp. 130–132

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Petroleum refining (continued)

Title	Author	Calculator	Reference
Speed of Hand-calculator Programs can be Improved	Stephen T. Kostecke	HP-67/97	*Oil Gas J.,* Vol. 78, Aug. 11, 1980, pp. 107–110
Shortcut Distillation Program Aids Design	Henry Y. Mak	TI-58/59	*Oil Gas J.,* Vol. 78, Oct. 20, 1980, pp. 138–141
Shortcut Program for Multicomponent Distillation	Mark Kesler	TI-58/59[b]	*Chem. Eng.,* Vol. 88, May 4, 1981, pp. 85–88.
Calculator Eases Flash Calculations	Chandra P. Verma	TI-58/59	*Oil Gas J.,* Vol. 79, Apr. 27, 1981, pp. 148–150
Rapid Calculator Solutions: ASTM/TBP; Other Probability Plot Problems	Tom D. Denchfield	HP-67/97	*Oil Gas J.,* Vol. 79, Apr. 27, 1981, pp. 179–184
Crude Dehydration/Desalting Calculations	Van B. Tran	HP-41C	*Oil Gas J.,* Mar. 15, 1982, pp. 76–79
Calculator Program Finds Petroleum Fraction Viscosities Over Wide Temperature Range	Gidion M. Barnea	HP-67/97	*Oil Gas.,* Vol. 80, May 10, 1982, pp. 148–150

Pipeline design and use

Title	Author	Calculator	Reference
Programmable Calculator Speeds Pipeline Span Computations	A. Marks	HP-67/97	*Oil Gas J.,* Vol. 76, Jan. 9, 1978, pp. 106–107
Hand-held Calculator Programs for Frequently Used Formulas Part 1: Williams-Hazen Pressure Drop	W. J. Turner	HP-67/97	*Pet. Eng. Int.,* Vol. 51, May 1979, pp. 84–90
Programmable Calculators Speed Gas-line Calculations	R. F. Parker	HP-67/97	*Oil Gas J.,* Vol. 77, May 7, 1979, pp. 67–72
Estimating Products Line Commingling	A. Marks	HP-67/97	*Oil Gas J.,* Vol. 77, Nov. 19, 1979, pp. 109–110
Pipeline Liquid Flow Problems Solved by Calculator	R. R. Burnett	HP-67/97	*Oil Gas J.,* Vol. 77, Nov. 19, 1979, pp. 134–152
Equation Programmed to Prompt: Weymouth	Dennis Cook	TI-58/59	*Oil Gas J.,* Vol. 77, Dec. 10, 1979, pp. 103–108
Equations Speed Permafrost-area Line Analysis	G. G. King	TI-58/59	*Oil Gas J.,* Vol. 78, Dec. 15, 1980, pp. 80–84
Program Solves Line Flow Equation	Kurt P. McCaslin	TI-58/59	*Oil Gas J.,* Vol. 79, Jan. 19, 1981, pp. 83–84
Equation Predicts Buried Pipeline Temperatures	Graeme G. King	TI-58/59	*Oil Gas J.,* Vol. 79, Mar. 16, 1981, pp. 65–72
Programs Speed Line Hydraulics	Lawrence K. Thummel	HP-41C	*Oil Gas J.,* Vol. 79, Apr. 20, 1981, pp. 76–85
Calculator Can Ease Pipeline Surge Analysis—Part 1	Mike Hein	Narrative, see next item	*Oil Gas J.,* Vol. 79, Aug. 10, 1981, pp. 100–106
Analyzing Line Surge with Hand-held Calculator—Part 2	Mike Hein	HP-41C	*Oil Gas J.,* Vol. 79, Aug. 17, 1981, pp. 128–134
Gas Pipeline Program Computes Five Variables	Steven R. Moore and Robert D. Huff	TI-58/59	*Oil Gas J.,* Vol. 80, Mar. 8, 1982, pp. 195–198
Programmable Calculator Uses Equation to Figure Steady-state Gas-Pipeline Flow	E. Holmberg	TI-58/59	*Oil Gas J.,* Vol. 80, Apr. 26, 1982, pp. 126–128

Insulation

Title	Author	Calculator	Reference
Calculator Program Analyzes Insulated Pipe	S. L. Barritt	HP-67/97	*Heat./Piping/Air Cond.,* Vol. 50, Mar. 1978, pp. 65–70
Program Calculates Heat Transfer through Composite Walls	Calvin R. Brunner	TI-58/59[a]	*Chem. Eng.,* Vol. 87, June 16, 1980, pp. 119–122
Calculating Heat Loss or Gain by an Insulated Pipe	Frank S. Schroder	HP-67/97[b]	*Chem. Eng.,* Vol. 89, Jan. 25, 1982, pp. 111–114
Heat Loss Through Insulated Steam Lines	J. G. Kloepfer and S. Dykstra	TI-58/59	*Oil Gas J.,* Vol. 80, Feb. 22, 1982, pp. 146–154

Pumps

Title	Author	Calculator	Reference
New Program Speeds Up Selection of Pumping Unit	Mark Seaman	TI-58/59	*Oil Gas J.,* Vol. 77, Nov. 12, 1979, pp. 226–229 (see next item)
New Program . . . Unit—A Correction	Mark Seaman	TI-58/59	*Oil Gas J.,* Vol. 77, Dec. 10, 1979, pp. 102
Rapid Calculation of Centrifugal-pump Hydraulics	W. Wayne Blackwell	TI-58/59[a]	*Chem. Eng.,* Vol. 87, Jan. 28, 1980, pp. 111–115
Calculator Program Computes Centrifugal Pump Efficiency	A. Marks	HP-67/97	*Oil Gas J.,* Vol. 78, Dec. 22, 1980, pp. 62–64
Gas Calculations Aid Submersible Pump Selections	John Beavers, others	TI-58/59	*Pet. Eng. Int.,* Vol. 53, July 1981, pp. 69–85

Sanitation, environment, and safety/health

Title	Author	Calculator	Reference
Sizing Force Mains for Economy	Louis Dancs	TI-58/59 & HP-67/97	*Water Sewage Works,* Vol. 124, Mar. 1977, pp. 84–86
Hydraulic Computations for Small Programmable Calculators	Thomas E. Croley II	TI-58/59 & HP-67/97	*Water Sewage Works,* Vol. 124, Nov. 1977, pp. 64–71
Computer Program for Open Channel Flow Calculation	Ralph Finch	TI-58/59	*Water Sewage Works Ref. Issue,* Vol. 125 Ref., 1978, pp. R:22–30

Sanitation, environment, and safety/health (continued)

Title	Author	Calculator	Reference
Predicting Sulfide in Force Mains	Karl E. Kienow and Kenneth K. Kienow	HP-67/97	*Water Sewage Works,* Vol. 125, Dec. 1978, pp. 48–49
Relative Humidity from Psychrometric Data	Åke Sison Stenius	HP-67/97	*Tappi,* Vol. 62, Apr. 1979, pp. 87–88
Programmed Approach to Water/Mass Analysis	George R. Spencer, Jr.	TI-58/59	*Pollut. Eng.,* Vol. 13, Feb. 1981, pp. 30–33
The Hand-held Programmable Calculator and the Occupational Safety and Health Practitioner: 1. TLV for Mixtures—Additive Effects. 2. TLV for Mixtures—Additive Effects: Liquid Source. 3. Time Weighted Average Exposure. 4. Time Weighted Average Exposure with Excursion Test. 5. Duct Sizing Calculations. 6. Computing Noise Dosage. 7. Converting Octave Band Sound Levels to A, B, or C Weighted Sound Pressure Levels. 8. Combining and Subtracting Sound Pressure Levels. 9. Cumulative Summing. 10. P Chart Computation. 11. C Chart Computation. 12. Pareto Analysis. 13. Work Injury Experience. 14. Concentration of an Air Contaminant from Sampling or Laboratory Data.	Leo Greenberg	TI-58/59	*Am. Ind. Hyg. Assoc. J.,* Vol. 42, Mar. 1981, pp. 165–177
Oxygen Transfer Parameter Estimation: 1. Complex Method. 2. Linearization Method	M. K. Stenstrom, others	TI-58/59	*ASCE, J. of Environ. Eng. Div.,* Vol. 107 (2), Apr. 1981, pp. 379–397
Psychrometric Analysis with a Programmable Calculator	Bernard N. DeWitt	TI-58/59	*Heat./Piping/Air Cond.,* Vol. 53, May 1981, pp. 59–62
Solve Psychrometric Problems with a Programmable Calculator	Theodore Atwood	TI-58/59	*Heat./Piping/Air Cond.,* Vol. 53, Dec. 1981, pp. 77–80
"Industrial Wastewater Treatment Plant Model	Kenneth A. Chacey and William S. McAvoy	HP-41C	*Pollut. Eng.,* Vol. 14, June, 1982, pp. 25–28

Piping

Title	Author	Calculator	Reference
Solving Engineering Problems on Programmable Pocket Calculators	Robert F. Benenati	HP-67/97[c]	*Chem. Eng.,* Vol. 84, Feb. 28, 1977, pp. 201–206 (see Refining for Part 2)
Versatile Calculator Program Eases Piping Design	Larry L. Simpson	HP-67/97[a]	*Chem. Eng.,* Vol. 86, Jan. 29, 1979, pp. 105–109 (see next item)
Versatile Calculator Program Eases Piping Design—Comment/Reply	Earle C. Smith	Narrative	*Chem. Eng.,* Vol. 86, Sept. 10, 1979, p. 5
Design Weld-neck Flanges Fast	John Stippick	TI-58/59	*Hydrocarbon Process.,* Vol. 59, May 1979, pp. 201–204
Steam Flow in Steel Pipes	T. S. Bryan and N. T. McLaury	HP-67/97	*Tappi,* Vol. 62, June 1979, pp. 91–92
Finding Economic Pipe Diameters Using Programmable Calculators	Neil Nebeker	TI-58/59	*Plant Eng.,* Vol. 33, June 14, 1979, pp. 150–153
Calculator Program Slashes Piping Analysis Time	M. Hassouneh and H. Bhaumik	HP-67/97	*Oil Gas J.,* Vol. 77, Oct. 29, 1979, pp. 167–172
Pressure Loss Through Valves	Kishan Bagadia	HP-67/97 and TI-58/59	*Plant Eng.,* Vol. 33, Oct. 31, 1979, p. 81
Friction Head Loss in Pipe	Kishan Bagadia	HP-67/97 and TI-58/59	*Plant Eng.,* Vol. 33, Oct. 31, 1979, p. 82
Analyze Fire Water Network by Calculator	H. Bhaumik	HP-67/97	*Oil Gas J.,* Vol. 77, Dec. 31, 1979, pp. 182–189
Versatile Program for Pressure-drop Calculations	James M. Meyer	HP-67/97[a]	*Chem. Eng.,* Vol. 87, Mar. 10, 1980, pp. 139–142
Program Finds Pressure Drop Through Pipe and Fittings	Barry L. Roth	TI-58/59	*Oil Gas J.,* Vol. 78, Mar. 24, 1980, pp. 168–170
Calculator Solves Pipe Flow Problems	Chandra P. Verma	TI-58/59	*Oil Gas J.,* Vol. 78, July 28, 1980, pp. 183–184
Pipe Friction Head Loss	Robert Bursey	TI-58/59	*Tappi,* Vol. 63, Nov. 1980, pp. 159–160
Program Calculates Two-phase Pressure Drop	W. Wayne Blackwell	TI-58/59	*Oil Gas J.,* Vol. 78, Nov. 24, 1980, pp. 116–124
Calculation of Drop Leg Performance	S. J. Dougherty	HP-67/97[a]	*Tappi,* Vol. 63, Dec. 1980, pp. 115–116
Equations Speed Permafrost-area Line Analysis	G. G. King	TI-58/59	*Oil Gas J.,* Vol. 78, Dec. 15, 1980, pp. 80–84
Program Solves Line Flow Equation	Kurt P. McCaslin	TI-58/59	*Oil Gas J.,* Vol. 79, Jan. 19, 1981, pp. 83–84
Piping Flexibility Analysis with a Programmable Calculator	Alfred D'Ambra	TI-58/59	*Heat./Piping/Air Cond.,* Vol. 53, May 1981, pp. 68–75
Program Sizes Pipe and Flare Manifolds for Compressible Flow	Paul Kandell	TI-58/59[b]	*Chem. Eng.,* Vol. 88, June 29, 1981, pp. 89–93
Solve Fluid Flow Problems with a Programmable Calculator	Theodore Atwood	TI-58/59	*Heat./Piping/Air Cond.,* Vol. 53, Sept. 1981, pp. 159–165
Calculating Two-phase Pressure Drop	W. Wayne Blackwell	TI-58/59[b]	*Chem. Eng.,* Vol. 88, Sept. 7, 1981, pp. 121–125
Pipe Branch Reinforcement Calculations	Alfred D'Ambra	TI-58/59	*Heat./Piping/Air Cond.,* Vol. 54, Feb. 1982, pp. 87–90

Piping (continued)

Title	Author	Calculator	Reference
Program Predicts Pressure Drop for Steam Flow	Calvin R. Brunner	TI-58/59[b]	*Chem. Eng.*, Vol. 89, Feb. 22, 1982, pp. 97–99
Sizing Condensate-return Lines	W. Wayne Blackwell	TI-58/59	*Chem. Eng.*, Vol. 89, July 12, 1982, pp. 105–108

Energy

Estimating Nuclear Fuel Cycle Cost Using a Hand-held Programmable Calculator	O. Wesley Taylor	TI-58/59	*Power Eng.*, Vol. 84, Feb. 1980, pp. 58–61
Using a Programmable Calculator for Energy Analysis	Gregory A. Specht	TI-58/59	*Plant. Eng.*, Vol. 34, Nov. 13, 1980, pp. 139–143
Estimate Solar Collector Size with a Programmable Calculator	M. D. Syed, others	TI-58/59	*Heat./Piping/Air Cond.*, Vol. 53, May 1981, pp. 81–85

Operations and maintenance

Finding Volume in Partially Filled Tanks	Erminio Santi	HP-67/97	*Chem. Eng.*, Vol. 86, June 18, 1979, pp. 144–147
Program Calculates Volumes of Partly Filled Vessels	W. Wayne Blackwell	TI-58/59	*Oil Gas J.*, Vol. 78, June 2, 1980, pp. 131–134
A Better Way to Balance Turbomachinery	L. Fielding and R. E. Mondy	TI-58/59	*Hydrocarbon Process.*, Vol. 60, Jan. 1981, pp. 97–104

Economic/financial

Fuel Savings in the Lime Kiln	S. Jagannath	TI-58/59	*Tappi*, Vol. 61, June 1978, pp. 83–84
Performing Cost-effective Analysis for Alternative Interceptor Sewer Designs	Karl E. Kienow and Kenneth K. Kienow	HP-67/97	*Water Sewage Works*, Vol. 125, Oct. 1978, pp. 43–48
Steam Savings in Multiple Effect Evaporator Systems	S. Jagannath	TI-58/59	*Tappi*, Vol. 61, Nov. 1978, pp. 123–124
Economics of Boiler Feedwater Heating	S. Jagannath	TI-58/59	*Tappi*, Vol. 62, Feb. 1979, pp. 89–90
Calculating Boiler Efficiency and Economics	Terry A. Stoa	TI-58/59[a]	*Chem. Eng.*, Vol. 86, July 16, 1979, pp. 77–81
Calculator Program Speeds Up Project Financial Analysis	David M. Kirkpatrick	TI-58/59[a]	*Chem. Eng.*, Vol. 86, Aug. 27, 1979, pp. 103–107
Hand-held Calculator Programs for Frequently Used Formulas: Discounted Cash Flow Projection with Price and Cost Escalation	W. J. Turner	HP-67/97	*Pet. Eng. Int.*, Vol. 52, Apr. 1980, pp. 76–94
Converting From Mechanical to Electrical Drives: The Looped Pointer Programming Method	S. Jagannath	TI-58/59	*Tappi*, Vol. 63, Nov. 1980, pp. 143–144
Program Calculates Stock-Options Tax	Ed Oxner	HP-67/97	*EDN*, Vol. 26, Feb. 4, 1981, p. 87
Calculators Quickly Find Tier I Revenue, Volume, WPT	Frank W. Lewis and Dipak K. Sinha	TI-58/59	*Oil Gas J.*, Vol. 79, March 16, 1981, pp. 80–84
Calculator Program Finds Present Value and Rate of Return on Investment Opportunities	Rene Santos	TI-58/59	*Oil Gas J.*, Vol. 79, Dec. 21, 1981, pp. 62–68
Calculator Program Aids Well Cost Management	Carey J. Doyle	TI-58/59	*Oil Gas J.*, Vol. 80, Jan. 18, 1982, pp. 111–116

Instrumentation and process control

Program Calculates Orifice Sizes for Gas Flow	William H. Mink	TI-58/59[a]	*Chem. Eng.*, Vol. 87, Aug. 25, 1980, pp. 91–94
TI-59 Program for Root Locus	G. Franklin	TI-58/59	*Electron. Eng.*, Vol. 53, Feb. 1981, pp. 25–27
Orifice Gas Flow Calculated Without Tables	Randy Freeman	TI-58/59	*Oil Gas J.*, Vol. 79, Mar. 9, 1981, pp. 156–161
Program Sizes Flange-top Orifice Plate	John E. Hogsett	TI-58/59	*Oil Gas J.*, Vol. 79, Mar. 23, 1981, pp. 132–136
Program Computes Orifice-meter Flow Rate	Jed R. Martin	TI-58/59	*Oil Gas J.*, Vol. 79, Oct. 12, 1981, pp. 130–131
Automatic Stability Calculations for Feedback Control Systems	Mehmet T. Gökbudak	HP-41C	*Control Eng.*, Vol. 29, June, 1982, pp. 80-82

Equipment engineering

Calculator Program Solves Cyclone Efficiency Equations	Yatendra M. Shah and Richard T. Price	TI-58/59[a]	*Chem. Eng.*, Vol. 85, Aug. 28, 1978, pp. 99–102
Overall Efficiency of a Combustion Boiler	S. Jagannath	TI-58/59	*Tappi*, Vol. 62, Jan. 1979, pp. 87–88

Equipment engineering (continued)

Title	Author	Calculator	Reference
Calculator Program for Sour-water Stripper Design	Norman H. Wild	HP-67/97[a]	*Chem. Eng.*, Vol. 86, Feb. 12, 1979, pp. 103–113
Calculator Program Aids Quench-tower Design	William H. Mink	TI-58/59[a]	*Chem. Eng.*, Vol. 86, Dec. 3, 1979, pp. 95–98
Program Predicts Radiant Heat Flux in Direct Fired Heaters	Tayseer A. Abdel-Halim	TI-58/59[a]	*Chem. Eng.*, Vol. 86, Dec. 17, 1979, pp. 87–91
Quick Calculation of Heat Exchanger Weight	Mike Taylor	HP-67/97	*Process Eng.*, Vol. 61, Jan. 1980, pp. 56–59
Calculator Analyzes Compressor Performance	Jim Urick and Fred Odom	TI-58/59	*Oil Gas J.*, Vol. 78, Jan. 14, 1980, pp. 60–65
Calculator Gives Compression Ratio for Compressors	Chandra P. Verma	TI-58/59	*Oil Gas J.*, Vol. 78, Feb. 25, 1980, pp. 128–130 (see next item)
Calculator Gives . . . Compressors—A Correction	Chandra P. Verma	TI-58/59	*Oil Gas J.*, Vol. 78, Mar. 31, 1980, p. 129
Kinetics of Fixed-bed Sorption Processes	Henry K. S. Tan	HP-67/97[a]	*Chem. Eng.*, Vol. 87, Mar. 24, 1980, pp. 117–119
Calculator Program for Designing Packed Towers	Vaclav I. Pancuska	TI-58/59[a]	*Chem. Eng.*, Vol. 87, May 5, 1980, pp. 113–114
Calculator Program Aids Design of Spouted Beds	Domingo Mele and Julian Martínez	HP-67/97[a]	*Chem. Eng.*, Vol. 87, Oct. 20, 1980, pp. 137–139
Calculating Hole-area Distribution for Liquid Spargers	William H. Mink	TI-58/59[a]	*Chem. Eng.*, Vol. 87, Nov. 17, 1980, pp. 277–281 (see next item)
Hole-area Distribution for Liquid Spargers—A Correction	William H. Mink	TI-58/59[a]	*Chem. Eng.*, Vol. 88, Apr. 6, 1981, pp. 93–95
Expansion Tank Calculations	M. D. Syed and D. G. Strang	TI-58/59	*Heat./Piping/Air Cond.*, Vol. 53, Jan. 1981, pp. 96–99
Coating Dryer Calculations	R. C. Walker	HP-67/97	*Tappi*, Vol. 64, Feb. 1981, pp. 119–121
Calculator Program for a Steam Condenser	Larry J. Haydu	HP-67/97[b]	*Chem. Eng.*, Vol. 87, Feb. 9, 1981, pp. 99–102
Using a Programmable Calculator to Solve Fan Law Problems	Joseph J. Loeffler	HP-67/97	*Plant Eng.*, Vol. 35, Mar. 19, 1981, pp. 167–170
A New Way to Rate an Existing Heat Exchanger	Rogerio G. Herkenhoff	HP-67/97/41C[b]	*Chem. Eng.*, Vol. 88, Mar. 23, 1981, pp. 213–215
Power Requirements of Pressurized Screens vs. Foil Frequency	R. M. Bach	TI-58/59	*Tappi*, Vol. 64, Aug. 1981, pp. 113–114
Calculating the Corrected LMTD in Shell & Tube Heat Exchangers	W. Wayne Blackwell	HP-67/97 & TI-58/59[b]	*Chem. Eng.*, Vol. 88, Aug. 24, 1981, pp. 101–106
Program Calculates Hydrocyclone Efficiency	Frank H. Merrill	HP-41C[b]	*Chem. Eng.*, Vol. 88, Nov. 2, 1981, pp. 71–78
Letters & Reply—Hydrocyclone Efficiency	R. L. Atwood	Narrative[d]	*Chem. Eng.*, Vol. 89, June 14, 1982, p. 5
Thermosyphon Reboiler Piping Designed by Computer	W. F. Abbott	TI-58/59	*Hydrocarbon Process.*, Vol. 61, Mar. 1982, pp. 127–129
Program Calculates Flame Temperature	Carl A. Vancini	HP-67/97[b]	*Chem. Eng.*, Vol. 89, Mar. 22, 1982, pp. 133–136
Solving Problems of Varying Heat-transfer Areas in Batch Processes	Maurizio Marzi	HP-41C	*Chem. Eng.*, Vol. 89, May 17, 1982, pp. 101–107

Chemical/physical properties

Calculate Enthalpy with a Pocket Calculator	Raymond T. Schneider	HP-67/97	*Chem. Eng.*, Vol. 84, May 23, 1977, pp. 145–152
Black Box for Pulp Streams	N. T. McLaury	HP-67/97	*Tappi*, Vol. 61, Sept. 1978, pp. 117–118
Calculating Roe Chlorine Number	S. Jagannath	TI-58/59	*Tappi*, Vol. 61, Dec. 1978, p. 93
Multi- or Single-sheet Light Scattering and Absorption Coefficients	A. Sison Stenius	HP-67/97	*Tappi*, Vol. 62, Jan. 1979, pp. 89–91 (see next item)
Multi- or Single-sheet . . . Coefficients—A Correction	Harold Peterson	HP-67/97	*Tappi*, Vol. 62, Mar. 1979, p. 109
Calculating Saturated Steam Temperature and Enthalpy of Vaporization	S. Jagannath	TI-58/59	*Tappi*, Vol. 62, Feb. 1979, pp. 89–90
Thermomechanical Pulp and Sheet Properties	S. Jagannath	TI-58/59	*Tappi*, Vol. 62, Mar. 1979, pp. 109–110
Predicting Volumes of Pure Liquids	James H. Weber	TI-58/59[a]	*Chem. Eng.*, Vol. 86, Mar. 26, 1979, pp. 173–177
Errata, correction to Predicting . . . Liquids by James H. Weber, in the March 29, 1979, issue of *Chemical Engineering*	Staff	TI-58/59[c]	*Chem. Eng.*, Vol. 86, June 18, 1979, p. 151
Specific Gravity of a Solid-Liquid Slurry	S. Jagannath	TI-58/59	*Tappi*, Vol. 62, Apr. 1979, p. 89
Kappa Number Calculation	Felipe Ramírez C.	TI-58/59	*Tappi*, Vol. 62, May 1979, p. 93
Color Analysis of Newsprint in the Dominant Wavelength Range: 570–585 nm	P. J. Mangin and M. B. Lyne	TI-58/59	*Tappi*, Vol. 62, May 1979, pp. 94–96
Predicting Volumes of Saturated Liquid Mixtures	James H. Weber	TI-58/59[a]	*Chem. Eng.*, Vol. 86, May 7, 1979, pp. 95–99
Calculator Gives Compressibility Factors	R. R. Burnett	HP-67/97	*Oil Gas J.*, Vol. 77, June 11, 1979, pp. 70–74
Predict the Viscosities of Pure Gases	James H. Weber	TI-58/59[a]	*Chem. Eng.*, Vol. 86, June 18, 1979, pp. 111–117
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A Programme for Compressible Flow	M. A. Taylor	SR-52	*Process. Eng.*, Vol. 57, Oct. 1976, pp. 83–84
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Gas and Vapor Concentration Calculations by Means of a Programmable Calculator	Marvin Weingast	SR-52	*Am. Ind. Hyg. Assoc. J.*, Vol. 38, Mar. 1977, pp. 147–148
Determining Ideal Stages on a Pocket Calculator	H. Tan	HP-25	*Chem. Eng.*, Vol. 84, Mar. 14, 1977, p. 154
More on Vaporization and Condensation	Edward Withee	SR-56	*Chem. Eng.*, Vol. 84, Sept. 26, 1977, pp. 121–122
Calculation of *J* Functions by a Pocket Calculator	H. Tan	HP-25	*Chem. Eng.*, Vol. 84, Oct. 24, 1977, p. 158
H-Factor Integration Program for HP-65 Calculator	J. E. Tasman	HP-65	*Tappi*, Vol. 61, May 1978, pp. 114–115
Another Approach—Amount of Inorganic Material in the Kraft Liquor Cycle	R. M. Samuals	HP-34C	*Tappi*, Vol. 63, Nov. 1980, pp. 145–146

Pumps

Determine System Head Curves With a Programmable Calculator	Louis Dancs	HP-25	*Water Sewage Works*, Vol. 124, Aug. 1977, pp. 61–63

Equipment engineering

Maximizing Economy in a Multiple Effect Evaporator	John A. Beaujean	HP-25	*Tappi*, Vol. 61, May 1978, pp. 113–114
Predicting Heat-exchanger Performance by Successive Summation	Robert A. Spencer, Jr.	SR-52[a]	*Chem. Eng.*, Vol. 85, Dec. 4, 1978, pp. 121–124

Equipment engineering (continued)

Title	Author	Calculator	Reference
Letters: Heat Exchange Program (Improves the program "Predicting Heat-exchanger Performance . . . Summation," by Robert A. Spencer, Jr., in the Dec. 4, 1978, issue of *Chemical Engineering*)	William Volk	SR-52[c]	*Chem. Eng.*, Vol. 86, June 18, 1979, p. 151
More on Calculating *H*-factors for Batch Digesters	R. M. Samuels	HP-34C	*Tappi*, Vol. 64, Mar. 1981, pp. 179–180
Heat Recovery in Counterflow Heat Exchangers: An Adaptation	R. M. Samuels	HP-34C	*Tappi*, Vol. 64, May 1981, pp. 131–132

Laboratory and clinical chemistry

Title	Author	Calculator	Reference
Molecular Calculations for Microanalysis on a Programmable Calculator: 1. Elemental Percentage Composition 2. Water Conversion	John M. Corliss	HP-65	*Microchem. J.*, Vol. 21, No. 4, Dec. 1976, pp. 458–465
Simple Methods for Calculating Reaction Equilibria in Single Reaction or Single Moiety Networks: 1. One Reaction Equilibrium—Stage 1 2. One Reaction Equilibrium—Stage 2	David J. M. Park	HP-25	*Comput. Programs Biomed.*, Vol. 6, Dec. 1976, pp. 263–268
Use of a Programmable Pocket Calculator in Processing Amino Acid Analysis Data	John H. Buchanan	HP-25	*J. Chromatog.*, Vol. 137, No. 2, 1977, pp. 475–480
Rapid, Rigorous Computation of Modulation Transfer Function on a Pocket Calculator	Peter M. Ronai and Dennis L. Kirch	HP-65	*J. Nucl. Med.*, Vol. 18, No. 6, June 1977, pp. 579–583
Crystallographic Computations on the Pocket Calculator: 1. Program to Calculate *d*-spacings for a Triclinic Unit Cell 2. d_{hkl} Spacings for a Monoclinic Cell 3. To Calculate Bond Distances for a Triclinic Unit Cell 4. To Calculate Torsion Angles	A. L. MacKay	HP-25	*J. Cryst. Mol. Struct.*, Vol. 9, No. 4, Dec. 1979, pp. 223–231
The Use of Programmable Calculators For the Calculation of Mass Median Diameter	H. W. West and D. L. Cashman	RS-EC4000	*Mosquito News*, Vol. 40, Dec. 20, 1980, pp. 631–632

Operations and maintenance

Title	Author	Calculator	Reference
Optimum Inventory? Do it With a Programmable Calculator	William I. Kaufman	SR-56	*Ind. Eng.*, Vol. 9, Apr. 1977, pp. 38–42
Fit Data to a Learning Curve Using a Programmable Calculator	Michael E. Richerson	SR-52	*Ind. Eng.*, Vol. 10, Jan. 1978, p. 23
HP-25 Program Makes Fast Cost Estimates	Joe Barocio	HP-25	*Electronics*, Vol. 52, Aug. 2, 1979, p. 138

Manufacturing

Title	Author	Calculator	Reference
Washer Efficiency Control by Use of the Displacement Ratio	Celso Hartkopf Lopes	HP-25	*Tappi*, Vol. 62, Sept. 1979, pp. 115–116
Programmable Calculators Simplify Balancing of Rotating Equipment	Stephen G. Scheneller	HP-33E	*Power*, Vol. 123, Dec. 1979, pp. 70–71
Finding Pipe Intersections	Thomas E. Andrako	HP-19C	*Mach. Des.*, Vol. 52, Feb. 7, 1980, p. 113
Cutting Pipe Intersections	Edward B. Becker	HP-65	*Mach. Des.*, Vol. 52, Apr. 10, 1980, pp. 133–134

Piping

Title	Author	Calculator	Reference
Calculator Programs Solve Fluid Flow Problems	F. Caplan	SR-52	*Heat./Piping/Air Cond.*, Vol. 50, Oct. 1978, pp. 85–87
Using Programmable Engineering Calculators for Fluid-Flow Problems	S. L. Barritt	SR-56	*Plant Eng.*, Vol. 32, Dec. 21, 1978, pp. 79–83
Analyzing Flashing Flow With a Programmable Calculator	Eugenio M. Amorante	SR-56	*Plant Eng.*, Vol. 33, Apr. 19, 1979, pp. 269–273

Piping (continued)

Title	Author	Calculator	Reference
Using the TI-57 to Calculate the Friction Factor	Mamerto A. Irasga	TI-57[a]	*Chem. Eng.*, Vol. 87, Apr. 21, 1980, pp. 129–130
Calc Program Finds Effective Flow Area	Uri Goldberg	HP-33E/C	*Mach. Des.*, Vol. 52, Oct. 9, 1980, p. 216
Calc Program Finds Gas Pressure Drop (Pressure Drop and Pipe Length)	Bruce M. Bailey	HP-29	*Mach. Des.*, Vol. 53, Jan. 8, 1981, pp. 162–164
Estimate of Economic Pipe Size	R. M. Samuels	HP-34C	*Tappi*, Vol. 64, June 1981, pp. 127–128

Instrumentation and process control

Solve Valve Sizing and Noise Calculations on Site in Minutes: 1. Sizing Calculation—Gas (scfh) 2. Sound Level Calculations—Standard Valves ($P_1/P_2 \geq 2.8$)	Kevin Hynes	HP-65	*Instrum. Control Syst.*, Vol. 49, Mar. 1976, pp. 43–47
Use of a Programmable Calculator to Determine Thermocouple Temperatures	W. G. Delinger	HP-25	*Solar Energy*, Vol. 20, Apr. 1978, pp. 359–360
Solving Instrumentation Problems With a Programmable Calculator: 1. Control Valve Sizing (Gas) 2. Orifice Sizing	P. S. Buckley and P. L. Mariam	HP-65	*Instrum. Technol.*, Vol. 22, Feb. 1979, pp. 31–37

Economic/financial

Program For Discounted Cash-flow Return on Investment	Norman H. Wild	HP-25	*Chem. Eng.*, Vol. 84, May 9, 1977, pp. 137–142
Simple Model for Determining Economic Feasibility of Processing New Oilseeds	G. C. Mistakas and K. D. Carlson	SR-56	*J. AM. Oil Chem. Soc.*, Vol. 56, Jan. 1979, pp. 29–32.

Insulation

Insulation Without Economics: 1. Bare Pipe Resistance 2. Insulation Thickness	M. McChesney and P. McChesney	TI-57	*Chem. Eng.*, Vol. 89, May 3, 1982, pp. 70–79

[a] Both HP and TI versions of this program appear in the book, "Calculator Programs for Chemical Engineers."
[b] Both HP and TI versions of this program appear in this book.
[c] This information appears in the book, "Calculator Programs for Chemical Engineers."
[d] This information appears in this book.

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Section II
Engineering Mathematics

Calculate statistics from a histogram

*Walter B. Thomas III**

☐ Experimental and process data are often recorded as a frequency distribution or histogram. For example, a quality inspector may record the range into which a measurement falls instead of recording the measured value. This calculator program, written for the HP-67/97 (and 19/29) calculators, finds the mean, variance and standard deviation of a distribution directly from the histogram.

How the program works

The program uses the frequency of observations in a cell (f_i) and the cell-midpoint values (x_i) to calculate the statistical parameters†:

Mean $\bar{x} = \Sigma f_i x_i / \Sigma f_i$

Variance $s^2 = [\Sigma f_i x_i^2 - ((\Sigma f_i x_i)^2/N)]/(N - 1)$

Standard deviation $s = \sqrt{s^2}$

Number of observations $N = \Sigma f_i$

Data (f_i, x_i) are entered, and accumulated in the memory registers. The program then calculates the statistical parameters, using two subroutines. There is also a subroutine that removes erroneous data pairs.

How to use the program

For the HP-67/97 calculators, enter the program as shown in Table I. Then follow the user instructions

*1501 Fishburn Rd., #5, Hershey, PA 17033.

†W. J. Dixon and F. J. Massey, Jr., "Introduction to Statistical Analysis," 3rd ed., McGraw-Hill, New York, 1969.

Program listing for HP-67/97 calculator — Table I

Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	023	X²	53
002	STO0	35 00	024	RCL1	36 01
003	X⇄Y	-41	025	÷	-24
004	ST+1	35-55 01	026	-	-45
005	X⇄Y	-41	027	RCL1	36 01
006	x	-35	028	1	01
007	ST+2	35-55 02	029	-	-45
008	RCL0	36 00	030	÷	-24
009	x	-35	031	R/S	51
010	ST+3	35-55 03	032	*LBLD	21 14
011	1	01	033	STO0	35 00
012	ST+4	35-55 04	034	X⇄Y	-41
013	RCL4	36 04	035	ST-1	35-45 01
014	R/S	51	036	X⇄Y	-41
015	*LBLB	21 12	037	x	-35
016	RCL2	36 02	038	ST-2	35-45 02
017	RCL1	36 01	039	RCL0	36 00
018	÷	-24	040	x	-35
019	R/S	51	041	ST-3	35-45 03
020	*LBLC	21 13	042	1	01
021	RCL3	36 03	043	ST-4	35-45 04
022	RCL2	36 02	044	R/S	51

To use this program on an HP-29 calculator, make the following changes: In step 001, replace ***LBL A** with ***LBL 1**; replace ***LBL B** in step 015 with two steps **GTO 1** and ***LBL 2**; replace ***LBL C** in step 020 with ***LBL 3**; replace ***LBL D** in step 032 with ***LBL 4**.

User instructions for HP-67/97 and HP-19/29 calculators — Table II

Step	Instructions	Input	HP 67/97 keys	Display	HP 19/29 keys
1	Enter program				
2	Initialize registers		**RTN** **f CL REG**		**g RTN** **f REG** **f STK**
3	Input data: cell frequency cell midpoint	f_i x_i	**ENTER** **A**	f_i Cell	**ENTER** **GTO 1 R/S**
4	Repeat step 3 for each cell				
5	Calculate the mean		**B**	$\bar{x}$	**GTO 2 R/S**
6	Calculate the variance		**C**	s^2	**GTO 3 R/S**
7	Calculate the standard deviation		$\sqrt{x}$	s	**f** $\sqrt{x}$
8	To remove an erroneous entry: input cell frequency input cell midpoint	 f_i x_i	 **ENTER** **D**	 f_i'	 **ENTER** **GTO 4 R/S**
9	To input a new distribution, go to step 2				

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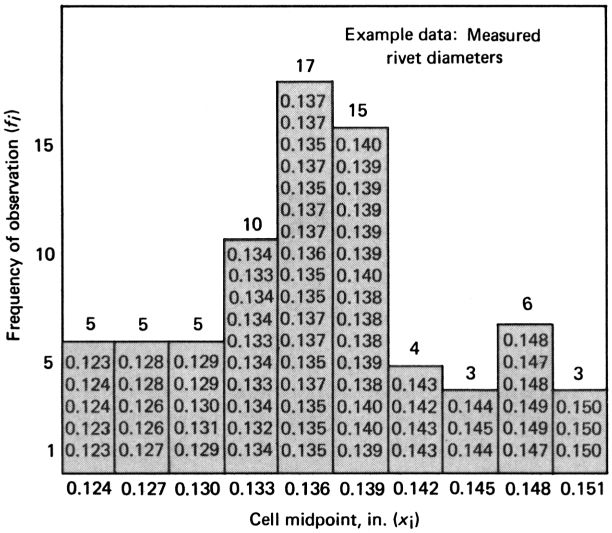
listed in Table II. (To run the program on the HP-19/29 calculators, make the changes noted in Tables I and II.)

Example: The figure shows the measured diameters of rivets leaving a machine shop—73 measurements overall, arranged in a histogram. Find the mean, variance and standard deviation of this distribution, using the HP-67/97 calculator program.



Solution: For each of the 10 cells, enter the frequency and cell midpoint as described in Table II. Press **B** to find $\bar{x}$. Press **C** to find s^2, and take the square root to find s. The results are:

Mean	$\bar{x} = 0.1367$ in.
Variance	$s^2 = 0.0000476$ in.^{2}
Standard deviation	$s = 0.00690$ in.

How does this compare with using the actual measured values to get the statistical parameters? If we had used all 73 data points, and calculated the parameters by conventional means, the results would have been: $\bar{x} = 0.1366$ in.; $s^2 = 0.0000479$ in.^{2}; $s = 0.00692$ in.

For TI users

A listing of the program for TI-58/59 is shown in Table III. User instructions are listed in Table IV.

Program listing for TI version **Table III**

Step	Code	Key	Step	Code	Key
000	76	LBL	041	33	X²
001	11	A	042	55	÷
002	42	STO	043	43	RCL
003	00	00	044	01	01
004	32	X⇌T	045	54	)
005	44	SUM	046	55	÷
006	01	01	047	53	(
007	65	×	048	43	RCL
008	32	X⇌T	049	01	01
009	95	=	050	75	−
010	44	SUM	051	01	1
011	02	02	052	54	)
012	65	×	053	95	=
013	43	RCL	054	91	R/S
014	00	00	055	76	LBL
015	95	=	056	14	D
016	44	SUM	057	42	STO
017	03	03	058	00	00
018	01	1	059	32	X⇌T
019	44	SUM	060	22	INV
020	04	04	061	44	SUM
021	43	RCL	062	01	01
022	04	04	063	65	×
023	91	R/S	064	32	X⇌T
024	76	LBL	065	95	=
025	12	B	066	22	INV
026	43	RCL	067	44	SUM
027	02	02	068	02	02
028	55	÷	069	65	×
029	43	RCL	070	43	RCL
030	01	01	071	00	00
031	95	=	072	95	=
032	91	R/S	073	22	INV
033	76	LBL	074	44	SUM
034	13	C	075	03	03
035	53	(	076	01	1
036	43	RCL	077	22	INV
037	03	03	078	44	SUM
038	75	−	079	04	04
039	43	RCL	080	91	R/S
040	02	02			

User instructions for TI program **Table IV**

Step	Instructions	Input	Key	Output
1	Load program	1	Feed side 1	1
2	Input data: cell frequency	f_i	x⇌t	
	cell midpoint	x_i	A	
3	Repeat step 2 for each cell			
4	Calculate the mean		B	$\bar{x}$
5	Calculate the variance		C	s^2
6	Calculate the standard deviation		$\sqrt{x}$	s
7	To remove an erroneous entry:			
	cell frequency	f_i'	x⇌t	
	cell midpoint	x_i'	D	

Nonlinear regression on a pocket calculator

This program for the Hewlett-Packard HP41C fits data to a user-defined function of several parameters, using a Gauss-Newton nonlinear-regression analysis. At least one memory module is required.

Brian W. Clare, Murdoch University

☐ We present here a review of curve-fitting procedures that reveals the value of nonlinear-regression techniques. A six-part program that makes use of the Gauss-Newton algorithm is described and the step-by-step running technique is detailed. An example is worked for the decomposition of available chlorine, and all relevant program printouts for this example are shown in tables.

Curve fitting

It is frequently desirable to represent data by an equation rather than a table. High-precision mathematical data are usually treated by interpolation formulas, which in effect fit exactly a polynomial of degree n to $n + 1$ points. This method produces completely unsatisfactory results when applied to data that may contain errors.

In this case, some form of regression analysis is better. This fits a formula, containing one or more parameters, to the data so that the sum of the squares of the residuals (the differences between the data values and the values predicted by the formula) is minimized.

If the form of the relationship between the dependent and independent variables is not known, polynomials of increasing degree may be used, until a satisfactory fit is obtained. Discontinuous or periodic data are better treated by a sum of trigonometric terms. Such approximations are linear in the parameters, which makes it particularly easy to fit them. However, these methods often require an excessive number of parameters, which makes them unsatisfactory.

Frequently, some relationship between the variables is known from theory or suspected from looking at the graphs. Such relationships may often be changed into a linear form. Eq. 1, for example, is transformed into Eq. 2 by taking logarithms of both sides:

$$y = ae^{bx} \tag{1}$$

$$\ln y = \ln a + bx \tag{2}$$

(The dependent variable y is related to the independent variable x by the parameters a and b.) The latter equation may then be treated by the methods of linear regression.

But such reduction is often not possible, nor even desirable. The transformation affects the weights assignable to the points in a complex, nonlinear, often undeterminable manner, thus distorting the resulting fit in a subtle but significant way.

Nonlinear regression

For these reasons, a better solution, often the only solution, is to apply the methods of nonlinear regression. While this has long been possible on a large computer, it has only recently become so on a personal calculator. The program described here is a development on earlier ones by the author [*1*] for the Hewlett-Packard HP67/97 and will run on the HP41C, a machine that is finding favor among engineers.

The method used is the Gauss-Newton algorithm [*2*] which, in the two-parameter case, works as follows:

Let there be points x_i, y_i that obey a relationship $y_i = f(x_i; \alpha, \beta) + \epsilon_i$ where α and β are parameters to be determined and ϵ_i are random errors. Then, if α_0, β_0 are first approximations to these parameters, better ones are given by α_1, β_1, where:

$$\alpha_1 = \alpha_0 - \delta\alpha$$
$$\beta_1 = \beta_0 - \delta\beta$$

$\delta\alpha$ and $\delta\beta$ are solutions to the linear equations:

$$\sum_i f_\alpha^2\,\delta\alpha + \sum_i f_\alpha f_\beta\,\delta\beta = \sum_i f f_\alpha$$

$$\sum_i f_\alpha f_\beta\,\delta\alpha + \sum_i f_\beta^2\,\delta\beta = \sum_i f f_\beta$$

and f_α and f_β are the partial derivatives of f with respect to α and β. In this program, the partial derivatives are obtained numerically:

$$f_\alpha = \frac{f(1.01\ \alpha, \beta; x) - f(\alpha, \beta; x)}{0.01\ \alpha}$$

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Routine INPUT allocates storage registers, handles data input, and can store data on cards **Table I**

```
01♦LBL "INPUT"
02 CLRG
03 CF 01
04 CF 02
05 "PRINT OR HALT ?"
06 AON
07 PROMPT
08 ASTO X
09 "HALT"
10 AOFF
11 ASTO Y
12 X=Y?
13 SF 02              Set Flag 2 if no
14 FIX 0              printer attached
15 "SIZE ?"
16 PROMPT
17 "⊢= "
18 ARCL X
19 AVIEW
20 1 E3
21 /
22 STO 09
23 "PARAMETERS ?"
24 PROMPT
25 "⊢= "
26 ARCL X
27 AVIEW
28 STO 07             Store number
29 "VARIABLES ?"      of parameters
30 PROMPT
31 "⊢= "
32 ARCL X
33 AVIEW
34 ST+ 09             Number of
35 "CONSTANTS ?"      variables and
36 PROMPT             constants
37 "⊢= "              Calculate
38 ARCL X             offset for
39 AVIEW              SYMLIN
40 ADV
41 RCL 07
42 ENTER↑
43 +
44 +
45 12
46 +
47 RCL 09
48 INT
49 +
50 STO 08             Offset for
51 XEQ 41             SYMLIN
52 STO 00
53 STO 02
54 XEQ 42
55 RCL 09
56 FRC
57 1 E3
58 *
59 RCL 08
60 -
61 RCL 09
62 INT
63 /
64 ENTER↑
65 ENTER↑
66 INT
67 X=Y?
68 DSE X
69 RCL 09
70 INT
71 *
72 RCL 08
73 +
74 1 E3
75 /
76 ST+ 00
77 RCL 00
78 STO 05
79 1
80 STO 03
81♦LBL 00
82 FIX 0              Input and
83 "X"                store variable
84 CF 29              in form xi <j>
85 ARCL 01            (input)
86 "⊢<"
87 ARCL 03
88 "⊢>= "
89 PROMPT
90 XEQ "FMT"
91 STO IND 00
92 ARCL X             Display or
93 SF 29              print data
94 AVIEW
95 ISG 00
96♦LBL 09
97 ISG 01
98 GTO 00
99 XEQ 42
100 ADV               Store Flag N
101 "N"               indicating to
102 ASTO IND 00       record next
103 ISG 00            card
104♦LBL 09
105 RCL 00
106 INT
107 RCL 09
108 INT
109 +
110 RCL 09
111 FRC
112 1 E3
113 *
114 X>Y?
115 GTO 07
116 GTO 05            Variable
117♦LBL 07           storage area
118 DSE 00            full
119♦LBL 09
120 ISG 03
121♦LBL 09
122 GTO 00
123♦LBL 05           Record data
124 DSE 00            card
125♦LBL 01
126 "RECORD: R/S"
127 PROMPT
128 RCL 02
129 RCL 09
130 FRC
131 +
132 WDTAX
133 SF 01             Set flag if
134 ISG 03            data card(s)
135♦LBL 09           recorded
136 RCL 05
137 STO 00
138 GTO 00
139♦LBL B
140 "APPROX"          Input starting
141 XEQ 43            approximation
142♦LBL 11
143 "P"
144 FIX 0
145 ARCL 01
146 "⊢ = "
147 PROMPT
148 XEQ "FMT"
149 STO IND 02
150 ARCL X
151 AVIEW
152 ISG 02
153♦LBL 09
154 ISG 01
155 GTO 11
156 ADV
157 "SOLVE"           Prompt for
158 PROMPT            next program
159♦LBL E            card
160 "END"             Insert Flag E
161 AVIEW             to indicate
162 CLX               end of data
163 "E"
164 ASTO IND 00
165 STOP
166 GTO 05
167♦LBL A            Change point
168 RCL 00
169 STO 10
170 RDN
171 STO 11
172 1
173 -
174 RCL 09
175 FRC
176 1 E3
177 *
178 RCL 02
179 -
180 2
181 -
182 RCL 09
183 INT
184 /
185 INT
186 MOD
187 RCL 09
188 INT
189 *
190 "CHANGE POINT"
191 AVIEW
192 STO 04
193 XEQ 41
194 +
195 STO 00
196 RCL 09
197 INT
198 1
199 STO 06
200 -
201 +
202 1 E3
203 /
204 ST+ 00
205♦LBL 70
206 "X"
207 CF 29
208 FIX 0
209 ARCL 06           xi
210 "⊢<"
211 ARCL 11
212 "⊢>= "            <j>
213 PROMPT
214 XEQ "FMT"
215 ARCL X
216 AVIEW             Print or display
217 STO IND 00        (corrected) X
218 1                 variable
219 ST+ 06
220 ISG 00
221 GTO 70
222 RCL 10
223 STO 00
224 ADV
225 GTO 01
226♦LBL 42
227 RCL 09
228 INT
229 1 E3
230 /
231 1
232 +
233 STO 01
234 RTN
235♦LBL 43
236 AVIEW
237 11
238 STO 02
239 1
240 RCL 07
241 1 E3
242 /
243 +
244 STO 01
245 RTN
246♦LBL 41
247 RCL 07
248 RCL 07
249 1
250 +
251 *
252 2
253 /
254 RCL 07
255 +
256 RCL 08
257 +
258 1
259 +
260 RTN
261 .END.
```

Routine SOLVE forms partial derivatives, sums squares and products, calls SYMLIN , and iterates **Table II**

```
♦LBL "SOLVE"
CF 00            Clear Flag 00 for
♦LBL 03          manual iteration
FS? 01
GTO 23
♦LBL 31
XEQ 41
STO 04
♦LBL 24
11
RCL 07
+
STO 05
RCL 09
INT
+
1
-
1 E3
/
ST+ 05
♦LBL 21
RCL IND 04       Copy next point
STO IND 05       into working area
ISG 04
♦LBL 09
ENTER↑
"E"
ASTO X
X=Y?             End of data?
GTO 20
CLX
"N"
ASTO X
X=Y?             Another data card?
GTO 23
ISG 05
GTO 21
GTO 22
♦LBL 23
XEQ 41
RCL 09
FRC
+
BEEP
RDTAX            Read data card
GTO 31
♦LBL 22
RCL 07
10
+
1 E3
/
11
+
STO 02
RCL 08
RCL 07
-
1
-
STO 03
XEQ "FUNC"       Calculate residual value
STO 10
♦LBL 02
1.01             Increase parameter
ST* IND 02       by 1%
XEQ "FUNC"       Recalculate residual
STO IND 03       value
1.01
ST/ IND 02       Return parameter to
RCL 10           its original value
ST- IND 03
RCL IND 02
1 E2
/
ST/ IND 03       Calculate partial
ISG 03           derivative
♦LBL 09
ISG 02
GTO 02           Next partial derivative
RCL 10
STO IND 03
RCL 08
STO 06
RCL 07
-
1
-
STO 02
RCL 08
1
-
1 E3
/
ST+ 02
RCL 02
STO 03
♦LBL 04
RCL IND 02       Calculate squares and
RCL IND 03       products of partial
*                derivatives, and sum
ST+ IND 06       them ready for SYMLIN
ISG 06
♦LBL 09
ISG 03
GTO 04
ISG 02
GTO 07
GTO 24
♦LBL 07
RCL 02
STO 03
GTO 04
♦LBL 20
XEQ "SYMLIN"     Solve linear system
0
STO 10
RCL 08
ENTER↑
ENTER↑
RCL 07
+
1
-
1 E3
/
+
STO 03
11
STO 02
0
♦LBL 06
RCL IND 03
ST- IND 02       Update parameter
RCL IND 02
/
ABS
+
ISG 02
♦LBL 09
ISG 03
GTO 06
FIX 5
VIEW X           Display and print
1 E-5            ε = Σ|δP/P|
X>Y?
GTO 05           Stop if ε < 10^-5
XEQ 41
2
-
1 E3
/
RCL 08
+
STO 05
0
♦LBL 25
STO IND 05       Clear summing
ISG 05           registers
GTO 25
TONE 9           Tone: iteration
TONE 9           completed
TONE 9
TONE 9
FC? 00
STOP             Stop if manually
GTO 03           iterating
♦LBL 41
RCL 07
RCL 07
1
+
*
2
/
RCL 07
+
RCL 08
+
1
+
RTN
♦LBL 05
"OUTPUT"         Finished; prompt for
PROMPT           output program card
RTN
♦LBL A
SF 00            Set Flag 00 for
GTO 03           automatic iteration
.END.
```

Routine SYMLIN, a program that solves symmetrical linear systems (up to 22x22 if used alone) **Table III**

```
01♦LBL "SYMLIN"
02 RCL 07        Transfer N
03 STO 00        and η
04 RCL 08
05 STO 01
06♦LBL C         Gaussian
07 RCL 01        elimination
08 STO 06
09 1
10 STO 02
11♦LBL 01
12 RCL 06
13 STO 03        i = 1
14 ISG 03
15♦LBL 09        No operation
16 RCL IND 03
17 RCL IND 01
18 /
19 STO 05
20 XEQ 08
21 STO 04
22 1
23 ST+ 02        m_ik = a_21/a_11
24 XEQ 08
25 1
26 -
27 1 E3
28 /
29 ST+ 04        Multiply top
30♦LBL 00        row by m_ik
31 RCL IND 03    and subtract
32 RCL 05        from Row k.
33 *
34 ST- IND 04
35 ISG 03
36♦LBL 09
37 ISG 04        Row finished?
38 GTO 00
39 1
40 ST+ 06
41 RCL 06
42 RCL 01
43 -
44 RCL 00
45 1
46 -
47 X≠Y?
48 GTO 01
49 RCL 00
50 1
51 +
52 ST+ 01
53 1
54 ST- 00
55 RCL 00
56 1
57 X≠Y?
58 GTO C         Start another
59 RCL 08        row
60 STO 01        Back
61 RCL 07        substitution
62 STO 00
63 STO 02
64 1
65 -
66 STO 06
67 1
68 STO 05        Column x, x_i
69 XEQ 08
70 1
71 -
72 STO 03
73 RCL IND 03    b_n
74 DSE 03
75 RCL IND 03    a_N,N
76 /
77 ISG 03
78♦LBL 09
79 STO IND 03
80 STO 04        x_N in R 04
81♦LBL A
82 RCL 06
83 STO 02
84♦LBL 03
85 XEQ 08        Multiply
86 1             column
87 -             by x_i
88 RCL 05
89 -
90 STO 03
91 RCL 04
92 ST* IND 03
93 DSE 02
94 GTO 03
95 DSE 06
96♦LBL 09
97 RCL 06
98 STO 02
99 XEQ 08
100 STO 03
101 1
102 ST+ 02       Prepare to
103 XEQ 08       sum row
104 2
105 -
106 1 E3
107 /
108 ST+ 03
109 RCL IND 03
110 STO 04
111 1
112 ST+ 03
113♦LBL 05
114 RCL IND 03
115 ISG 03
116 GTO 07       Sum a_ij x_j
117 GTO 06
118♦LBL 07
119 ST+ IND 03
120 GTO 05
121♦LBL 06
122 ST- IND 03   Subtract from
123 RCL 04       from b_i
124 ST/ IND 03
125 RCL IND 03
126 STO 04
127 RCL 06
128 X=0?
129 GTO D
130 1
131 ST+ 05       Next column
132 GTO A
133♦LBL D
134 RCL 00
135 STO 02       Shift solution
136 RCL 01       to first row
137 +
138 1
139 -
140 STO 04       Address of x_N
141♦LBL 11
142 XEQ 08
143 1
144 -
145 STO 03
146 RCL IND 03   Transfer
147 STO IND 04
148 DSE 04
149♦LBL 09
150 DSE 02
151 GTO 11
152 RTN
153♦LBL 08      Calculate
154 RCL 00       address of
155 1.5          end of row
156 +
157 RCL 02
158 2
159 /
160 -
161 RCL 02
162 *
163 RCL 01
164 +
165 RTN
166 .END.
```

Routine OUTPUT prints out the parameters, the residuals and the standard deviation **Table IV**

```
01♦LBL "OUTPUT"
02 ADV
03♦LBL C
04 "SOLUTION:"
05 XEQ 43
06♦LBL 12
07 "P"
08 FIX 0
09 ARCL 01
10 "⊢ = "
11 RCL IND 02
12 XEQ "FMT"
13 ARCL X        Print and display parameter
14 AVIEW
15 FS? 02
16 STOP          Stop and display parameter
17 ISG 02        if printer not attached
18♦LBL 09
19 ISG 01
20 GTO 12        Next parameter
21 1
22 STO 06
23 0
24 STO 10
25♦LBL "R"
26 ADV
27 "RESIDUALS"
28 AVIEW
29 FS? 01
30 GTO 53        Read data card, if
31♦LBL 61       cards used
32 XEQ 41
33 STO 04
34♦LBL 54
35 11
36 RCL 07        Prepare R 05 for indirect
37 +             store of variables
38 STO 05
39 RCL 09
40 INT
41 +
42 1
43 -
44 1 E3
45 /
46 ST+ 05
47♦LBL 51
48 RCL IND 04    Copy variables into
49 STO IND 05    working area
50 ISG 04
51♦LBL 09
```

(Continued on next page)

(Continued) Table IV

```
52 ENTER↑
53 "E"
54 ASTO X
55 X=Y?        Last residual?
56 GTO 50
57 CLX
58 "N"
59 ASTO X
60 X=Y?        Another card?
61 GTO 53
62 ISG 05
63 GTO 51      Next variable
64 GTO 52
65♦LBL 53
66 XEQ 41
67 RCL 09
68 FRC
69 +
70 BEEP
71 RDTAX       Read next data card
72 GTO 61
73♦LBL 52
74 RCL 07
75 10
76 +
77 1 E3
78 /
79 11
80 +
81 STO 02
82 RCL 08
83 RCL 07
84 -
85 1
86 -
87 STO 03
88 "R"
89 FIX 0
90 ARCL 06     Identification number
91 "⊢:  "      of residual
92 XEQ "FUNC"  Calculate and format
93 XEQ "FMT"   residual
94 ARCL X
95 AVIEW       Print or display residual
96 FS? 02
97 STOP        Stop if printer not
98 X↑2         attached
99 ST+ 10      Square and accumulate
100 1          residual
101 ST+ 06     Count points
102 GTO 54     Next residual
103♦LBL 50
104 RCL 10     Calculate standard
105 RCL 06     deviation
106 RCL 09
107 INT
108 -
109 1
110 -
111 /
112 SQRT
113 ADV
114 "SDEV = "  Print standard deviation
115 XEQ "FMT"
116 ARCL X
117 AVIEW
118 ADV
119 ADV
120 ADV
121 ADV
122 ADV
123 STOP       Finished
124♦LBL 42
125 RCL 09
126 INT
127 1 E3
128 /
129 1
130 +
131 STO 01
132 RTN
133♦LBL 43
134 AVIEW
135 11
136 STO 02
137 1
138 RCL 07
139 1 E3
140 /
141 +
142 STO 01
143 RTN
144♦LBL 41
145 RCL 07     Prepare for indirect
146 RCL 07     recall of variables from
147 1          point storage
148 +
149 *
150 2
151 /
152 RCL 07
153 +
154 RCL 08
155 +
156 1
157 +
158 RTN
159 .END.
```

Available chlorine deteriorates after production **Table V**

Length of time since produced, weeks X	Available chlorine, % Y	Average Y, % $\bar{Y}$	Predicted Y, using the model $\hat{Y}$
8	0.49, 0.49	0.490	0.490
10	0.48, 0.47, 0.48, 0.47	0.475	0.472
12	0.46, 0.46, 0.45, 0.43	0.450	0.457
14	0.45, 0.43, 0.43	0.437	0.445
16	0.44, 0.43, 0.43	0.433	0.435
18	0.46, 0.45	0.455	0.427
20	0.42, 0.42, 0.43	0.423	0.420
22	0.41, 0.41, 0.40	0.407	0.415
24	0.42, 0.40, 0.40	0.407	0.410
26	0.41, 0.40, 0.41	0.407	0.407
28	0.41, 0.40	0.405	0.404
30	0.40, 0.40, 0.38	0.393	0.401
32	0.41, 0.40	0.405	0.399
34	0.40	0.400	0.397
36	0.41, 0.38	0.395	0.396
38	0.40, 0.40	0.400	0.395
40	0.39	0.390	0.394
42	0.39	0.390	0.393

The program

The program is semi-interactive and consists of six parts:

1. Routine INPUT (Table I), which allocates registers for storage, and handles input of data into registers and, if necessary, storage of data on magnetic cards.
2. Routine SOLVE (Table II), which forms the partial derivatives and their sums of squares and sums of products, calling SYMLIN to solve the linear equation system, implementing the corrections to the parameters, and returning for further iteration.
3. Routine SYMLIN (Table III), a program that solves symmetrical linear systems (up to 22 × 22 if used alone).
4. Routine FUNC, the user-written program that evaluates the residuals whose sum of squares is to be minimized.
5. Routine FMT, a short program that determines the format of the output (see Table I).
6. Routine OUTPUT (Table IV), which prints out the parameters, the residuals and the standard deviation.

The necessary requisites are the HP41C and at least one memory module. The cardreader is also needed since running the program without it would be tedious (though possible). The program is designed to work with or without the printer. The size of the problem that can be handled is determined by the number of memory modules used, by FUNC and FMT (which are written by the user), and by SOLVE and SYMLIN, which together occupy 585 bytes.

The INPUT program reserves space for intermediate calculations (R_{00} to R_{10} plus a set equal to one greater than the number of parameters), as well as for the parameters, variables and constants (which may be partitioned in any way desired), and for the matrix of coefficients of the linear equation system. The remainder is available for the data. With simple cases, more than enough space for 100 points is available. This may be expanded indefinitely by storing data on cards.

Running the program

Follow these steps, with the HP41C in the USER mode throughout:

1. Write and store the program FUNC, assuming that the parameters to be adjusted are in R11 to R($10+P$), the variables in R($11+P$) to R($10+P+V$), and the constants in R($11+P+V$) to R($10+P+V+C$). P, V and C are, respectively, the number of parameters, variables and constants. The program should return the value of the residual to the X register.

2. Write and store the program FMT, which determines the format in which numbers are to be printed. Example: LBL "FMT," SCI5, END.

3. Execute (SIZE) as follows: Determine the number of bytes in programs FMT and FUNC; subtract these from the total number of bytes in the calculator configuration used; subtract also 585 (the number of bytes in SOLVE plus SYMLIN); divide by seven and take the integer part. This is the size.

4. Press [GTO] . . , retaining FUNC and FMT, then load program INPUT. Proceed as follows:

Key in	Press	Response
	[XEQ] (INPUT)	'PRINT OR HALT?'
(PRINT) if printer is to be used; (HALT) otherwise	[R/S]	'SIZE?'
Size (as determined)	[R/S]	'PARAMETERS?'
Number of parameters	[R/S]	'VARIABLES?'
Number of variables	[R/S]	'CONSTANTS?'
Number of constants	[R/S]	X1<1> =

For the purposes of the program, the variables x and y are labelled X1 and X2. The ith data point is labelled X1(i), X2(i). Input data as prompted—X1(1) = , X2(1) = , etc.—terminating each value by [R/S].

Continue until all data are input or until input is interrupted by the display 'RECORD : R/S.' If this happens, it means that the memory is full and the data must be recorded on cards if there are any more points. If there are no more points, press [E]. The calculator responds 'END.' (Here, the top five keys are referred to by their ALPHA designations when in the USER mode.)

Erroneous points may then be corrected thus: Key in the point number and press [A]. The calculator then prompts for the X values for that point. Key them in, terminating each with [R/S]. When the data entry for the point is finished, the calculator responds

FUNC evaluates residuals; FMT formats the output **Table VI**

```
01♦LBL "FUNC"    08 E↑X       15 RCL 14
02 RCL 13        09 RCL 16    16 -
03 RCL 15        10 RCL 11    17 RTN
04 -             11 -         18♦LBL "FMT"
05 RCL 12        12 *         19 FIX 4
06 *             13 RCL 11    20 END
07 CHS           14 +
```

'RECORD : R/S.' If there are no more points, press [B]. If there are, press [R/S] and pass blank cards to record the data, and resume data entry as prompted.

On conclusion of data entry, press [E] and, if cards have been recorded, [R/S], [R/S], and pass the final data cards.

5. When data entry is complete, store the values of any constants (e.g., C1[STO]15, C2[STO]16, . . .).

6. Press [B]. The calculator prompts for the starting approximation to the parameters. Enter each, followed by [R/S]. Display then reads 'SOLVE.'

7. Clear program INPUT and load SOLVE. Press [GTO] . . . Load SYMLIN.

8. [XEQ] SOLVE.

If data have been recorded on cards, [BEEP] will sound and 'CARD' will appear in the display. Read the data cards in the order in which they were recorded, on successive such prompts.

When all the data have been entered, and the first iteration is complete, four tones will sound and the machine will halt, displaying a number that is $\epsilon = \sum \left| \frac{\delta x_i}{x_i} \right|$ and is a measure of the proximity of the solution. If this is less than approximately 1, another iteration may be initiated by pressing [R/S]; alternatively, pressing [A] will cause the machine to iterate automatically until $\epsilon < 10^{-5}$.

If ϵ is large, divergence may be occurring and the solution should be inspected ([RCL]11, [RCL]12, . . .) to see whether it is reasonable. If necessary, 'unreasonable' parameters can be changed manually—e.g., NEW VALUE, STO 11, and so on.

When convergence has occurred, the display will read 'OUTPUT.'

9. Clear programs SOLVE and SYMLIN. Enter program OUTPUT. [XEQ] OUTPUT. If the machine was instructed to (PRINT), the output follows: P1 = (first parameter), P2 = (second parameter); then R1:, R2:, etc. (the values of the residuals); and finally SDEV = (the standard deviation). If the machine was instructed to (HALT) (e.g., if there were no printer attached), it is necessary to press [R/S] to obtain each output. (Correction: Program FUNC should end RCL14, −, CHS, END.)

Decomposition of available chlorine

An example of nonlinear regression in the chemical industry was given by H. Smith and S. D. Dubey [3]. A

Executing INPUT (data) and OUTPUT (solution) **Table VII**

```
SIZE ?= 230.
PARAMETERS ?= 2.
VARIABLES ?= 2.
CONSTANTS ?= 2.

X1(1)= 8.0000
X2(1)= 0.4900

X1(2)= 8.0000
X2(2)= 0.4900

X1(3)= 10.0000
X2(3)= 0.4900

X1(4)= 10.0000
X2(4)= 0.4700

X1(5)= 10.0000
X2(5)= 0.4800

X1(6)= 10.0000
X2(6)= 0.4700

X1(7)= 12.0000
X2(7)= 0.4600

X1(8)= 12.0000
X2(8)= 0.4600

X1(9)= 12.0000
X2(9)= 0.4500

X1(10)= 12.0000
X2(10)= 0.4300

X1(11)= 14.0000
X2(11)= 0.4500

X1(12)= 14.0000
X2(12)= 0.4300

X1(13)= 14.0000
X2(13)= 0.4300

X1(14)= 16.0000
X2(14)= 0.4400

X1(15)= 16.0000
X2(15)= 0.4300

X1(16)= 16.0000
X2(16)= 0.4300

X1(17)= 18.0000
X2(17)= 0.4600

X1(18)= 18.0000
X2(18)= 0.4500

X1(19)= 20.0000
X2(19)= 0.4200

X1(20)= 20.0000
X2(20)= 0.4200

X1(21)= 20.0000
X2(21)= 0.4300

X1(22)= 22.0000
X2(22)= 0.4100

X1(23)= 22.0000
X2(23)= 0.4100

X1(24)= 22.0000
X2(24)= 0.4000

X1(25)= 24.0000
X2(25)= 0.4200

X1(26)= 24.0000
X2(26)= 0.4000

X1(27)= 24.0000
X2(27)= 0.4000

X1(28)= 26.0000
X2(28)= 0.4100

X1(29)= 26.0000
X2(29)= 0.4000

X1(30)= 26.0000
X2(30)= 0.4100

X1(31)= 28.0000
X2(31)= 0.4100

X1(32)= 28.0000
X2(32)= 0.4000

X1(33)= 30.0000
X2(33)= 0.4000

X1(34)= 30.0000
X2(34)= 0.4000

X1(35)= 30.0000
X2(35)= 0.3800

X1(36)= 32.0000
X2(36)= 0.4100

X1(37)= 32.0000
X2(37)= 0.4000

X1(38)= 34.0000
X2(38)= 0.4000

X1(39)= 36.0000
X2(39)= 0.4100

X1(40)= 230.0000
X2(40)= 0.3800

X1(41)= 38.0000
X2(41)= 0.4000

X1(42)= 38.0000
X2(42)= 0.4000

X1(43)= 40.0000
X2(43)= 0.3900

X1(44)= 42.0000
X2(44)= 0.3900

END
CHANGE POINT
X1(40)= 36.0000
X2(40)= 0.3800

APPROX
END
APPROX
P1 = 0.2500
P2 = 0.1000
     0.36584
     0.00939
     0.00023
     0.00001

SOLUTION:
P1 = 0.3901
P2 = 0.1016

RESIDUALS
R1:   0.0000
R2:   0.0000
R3:  -0.0084
R4:   0.0016
R5:  -0.0084
R6:   0.0016
R7:  -0.0034
R8:  -0.0034
R9:   0.0066
R10:  0.0266
R11: -0.0056
R12:  0.0144
R13:  0.0144
R14: -0.0056
R15:  0.0044
R16:  0.0044
R17: -0.0337
R18: -0.0237
R19: -0.0004
R20: -0.0004
R21: -0.0104
R22:  0.0042
R23:  0.0042
R24:  0.0142
R25: -0.0102
R26:  0.0098
R27:  0.0098
R28: -0.0038
R29:  0.0062
R30: -0.0038
R31: -0.0068
R32:  0.0032
R33:  0.0008
R34:  0.0008
R35:  0.0208
R36: -0.0111
R37: -0.0011
R38: -0.0027
R39: -0.0141
R40:  0.0159
R41: -0.0051
R42: -0.0051
R43:  0.0040
R44:  0.0033

SDEV = 0.0109
```

certain product was required to have a fraction 0.50 available chlorine at the time of manufacture. The product reaches the market in eight weeks, during which time the available chlorine has fallen to 0.49. After this time, non-constant storage conditions lead to a dispersed decomposition rate. It is, however, desirable to have some means of predicting the available chlorine at future intervals in order to determine how long the material should be kept before being discarded.

A number of determinations of available chlorine at different times after manufacture are shown in Table V. It was known that the available chlorine fell to about half its original value on prolonged storage. A nonlinear model, based on first-order kinetics, was postulated as follows:

$$Y = \alpha + (0.49 - \alpha)e^{-\beta(X-8)} \qquad \ldots 3$$

where Y is the fraction of available chlorine X weeks from manufacture.

The program FUNC, corresponding to Eq. 3, together with program FMT, is shown in Table VI. A value of 0.25 was chosen for α, and by trial with several points, a value of 0.1 for β. Registers were allocated:

α ($P1$) in R11
β ($P2$) in R12
x_i ($X1$) in R13
y_i ($X2$) in R14
8 in R15
0.49 in R16

(The constants could have as easily been written into program memory.)

The output from the program, run with the printer, is shown in Table VII. The solution is $\alpha = 0.3901$, $\beta = 0.1016$. The residuals are as shown in Table VII.

For TI-58/59 users

The TI program listing is contained in Table VIII, and user instructions are offered in Table IX. The printout of the example given in the text is shown in Table X.

Program listing for TI version **Table VIII**

Step	Code	Key	Step	Code	Key
000	76	LBL	016	91	R/S
001	11	A	017	76	LBL
002	87	IFF	018	22	INV
003	01	01	019	69	OP
004	22	INV	020	20	20
005	86	STF	021	72	ST*
006	01	01	022	00	00
007	42	STO	023	69	OP
008	16	16	024	20	20
009	32	X:T	025	32	X:T
010	42	STO	026	72	ST*
011	17	17	027	00	00
012	01	1	028	91	R/S
013	07	7	029	76	LBL
014	42	STO	030	12	B
015	00	00	031	22	INV

(Continued) Table VIII

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
032	86	STF	095	95	=	158	10	10	221	08	08	284	42	STO
033	01	01	096	22	INV	159	43	RCL	222	94	+/-	285	08	08
034	43	RCL	097	49	PRD	160	09	09	223	85	+	286	42	STO
035	00	00	098	06	06	161	33	X^2	224	43	RCL	287	10	10
036	42	STO	099	43	RCL	162	44	SUM	225	07	07	288	42	STO
037	15	15	100	06	06	163	11	11	226	95	=	289	11	11
038	43	RCL	101	65	×	164	43	RCL	227	55	÷	290	42	STO
039	03	03	102	43	RCL	165	09	09	228	43	RCL	291	12	12
040	42	STO	103	05	05	166	65	×	229	12	12	292	43	RCL
041	01	01	104	95	=	167	43	RCL	230	95	=	293	03	03
042	43	RCL	105	44	SUM	168	06	06	231	42	STO	294	42	STO
043	04	04	106	07	07	169	95	=	232	14	14	295	01	01
044	42	STO	107	43	RCL	170	44	SUM	233	43	RCL	296	43	RCL
045	02	02	108	06	06	171	12	12	234	01	01	297	04	04
046	01	1	109	33	X^2	172	43	RCL	235	75	-	298	42	STO
047	06	6	110	44	SUM	173	02	02	236	43	RCL	299	02	02
048	42	STO	111	08	08	174	42	STO	237	13	13	300	01	1
049	00	00	112	43	RCL	175	04	04	238	95	=	301	06	6
050	76	LBL	113	01	01	176	43	RCL	239	42	STO	302	42	STO
051	25	CLR	114	42	STO	177	15	15	240	03	03	303	00	00
052	71	SBR	115	03	03	178	32	X⇄T	241	43	RCL	304	61	GTO
053	15	E	116	01	1	179	43	RCL	242	02	02	305	25	CLR
054	69	OP	117	93	.	180	00	00	243	75	-	306	76	LBL
055	20	20	118	00	0	181	67	EQ	244	43	RCL	307	14	D
056	73	RC*	119	01	1	182	32	X⇄T	245	14	14	308	00	0
057	00	00	120	49	PRD	183	69	OP	246	95	=	309	42	STO
058	94	+/-	121	04	04	184	20	20	247	42	STO	310	06	06
059	42	STO	122	69	OP	185	61	GTO	248	04	04	311	42	STO
060	05	05	123	30	30	186	25	CLR	249	43	RCL	312	07	07
061	32	X⇄T	124	71	SBR	187	76	LBL	250	13	13	313	42	STO
062	44	SUM	125	15	E	188	32	X⇄T	251	55	÷	314	08	08
063	05	05	126	69	OP	189	53	(	252	43	RCL	315	01	1
064	01	1	127	20	20	190	43	RCL	253	03	03	316	06	6
065	93	.	128	73	RC*	191	07	07	254	95	=	317	42	STO
066	00	0	129	00	00	192	55	÷	255	50	I×I	318	00	00
067	01	1	130	94	+/-	193	43	RCL	256	85	+	319	76	LBL
068	49	PRD	131	42	STO	194	12	12	257	53	(	320	42	STO
069	03	03	132	09	09	195	75	-	258	43	RCL	321	71	SBR
070	69	OP	133	43	RCL	196	43	RCL	259	14	14	322	15	E
071	30	30	134	05	05	197	10	10	260	55	÷	323	69	OP
072	71	SBR	135	22	INV	198	55	÷	261	43	RCL	324	20	20
073	15	E	136	44	SUM	199	43	RCL	262	04	04	325	73	RC*
074	69	OP	137	09	09	200	11	11	263	95	=	326	00	00
075	20	20	138	32	X⇄T	201	54	)	264	50	I×I	327	42	STO
076	73	RC*	139	44	SUM	202	55	÷	265	54	)	328	06	06
077	00	00	140	09	09	203	53	(	266	95	=	329	32	X⇄T
078	94	+/-	141	43	RCL	204	43	RCL	267	42	STO	330	22	INV
079	42	STO	142	02	02	205	08	08	268	12	12	331	44	SUM
080	06	06	143	65	×	206	55	÷	269	32	X⇄T	332	06	06
081	43	RCL	144	93	.	207	43	RCL	270	01	1	333	43	RCL
082	05	05	145	00	0	208	12	12	271	52	EE	334	06	06
083	22	INV	146	01	1	209	75	-	272	94	+/-	335	33	X^2
084	44	SUM	147	95	=	210	43	RCL	273	05	5	336	44	SUM
085	06	06	148	22	INV	211	12	12	274	77	GE	337	08	08
086	32	X⇄T	149	49	PRD	212	55	÷	275	14	D	338	43	RCL
087	44	SUM	150	09	09	213	43	RCL	276	32	X⇄T	339	15	15
088	06	06	151	43	RCL	214	11	11	277	22	INV	340	32	X⇄T
089	43	RCL	152	09	09	215	54	)	278	52	EE	341	43	RCL
090	01	01	153	65	×	216	95	=	279	99	PRT	342	00	00
091	65	×	154	43	RCL	217	42	STO	280	91	R/S	343	67	EQ
092	93	.	155	05	05	218	13	13	281	00	0	344	43	RCL
093	00	0	156	95	=	219	65	×	282	42	STO	345	69	OP
094	01	1	157	44	SUM	220	43	RCL	283	07	07	346	20	20

(Continued) Table VIII

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
347	61	GTO	360	05	5	373	99	PRT	386	75	-	399	04	4
348	42	STO	361	54	)	374	43	RCL	387	08	8	400	09	9
349	76	LBL	362	65	×	375	04	04	388	95	=	401	75	-
350	43	RCL	363	02	2	376	99	PRT	389	65	×	402	43	RCL
351	53	(	364	54	)	377	98	ADV	390	43	RCL	403	03	03
352	43	RCL	365	34	√X	378	43	RCL	391	04	04	404	54	)
353	08	08	366	42	STO	379	06	06	392	94	+/-	405	85	+
354	55	÷	367	06	06	380	99	PRT	393	95	=	406	43	RCL
355	53	(	368	22	INV	381	91	R/S	394	22	INV	407	03	03
356	43	RCL	369	52	EE	382	76	LBL	395	23	LNX	408	95	=
357	00	00	370	98	ADV	383	15	E	396	65	×	409	32	X⇌T
358	75	-	371	43	RCL	384	73	RC*	397	53	(	410	92	RTN
359	01	1	372	03	03	385	00	00	398	93	.			

User instructions for TI version **Table IX**

The TI program requires the nonlinear function to be entered as subroutine E, starting at line 382. (The program listing in Table VIII has the text function—Eq. 3—in this location.) Because of size limitations, the nonlinear function may have only two variable parameters, α and β in the text. The calculated values of these parameters are stored in registers 03 and 04 by the program. The first estimates of the parameters are made by the engineer, and are placed in registers 03 and 04 before the start of the program. (The first estimates in the text example are 0.25 and 0.1.)

Also because of size limitation, only a maximum of 22 pairs of *y-x* values can be handled. The program uses 16 storage registers for the calculations, and the 22 pairs of *x-y* values must be stored, requiring a total of 60 storage areas.

Program operation is as follows:

1.The nonlinear function is entered in place of the material following line 385 in the program listed. Lines 386 to 479 are available for the function. (Be sure to end with a **RETURN** instruction.)

2.The preliminary estimate of the function parameters is entered in storage registers 03 and 04 (i.e., for the example, enter the initial value for α as 0.25 STO 03, and for β of 0.1 as 0.1 STO 04). Y-X data are entered as:

Y, key **X↔T**

X, key **A**

3. When all the data are entered, key **B** gives an estimate of the solution: ϵ in the text. This calculation may take a few minutes.

Additional estimates may be automatically made by using key **R/S.** If the estimate is satisfactory, key **D** will give the values of the parameters. If the ϵ value is less than 1E-5, the program automatically goes to key **D** and calculates the parameters.

Key **D** gives the values of two parameters in the nonlinear function, first the value of α in register 03, and then the value of β in 04. It then gives the goodness of fit, measured as the standard deviation—the square root of the mean of the sums of the squares of deviation. The printout of the example is shown in Table X.

Example for TI version **Table X**

.3841288375	Estimates for ϵ
.0399996648	
.0010715053	
.0000234167	
.3882936306	α
.0935055038	β
.0079845881	Standard deviation

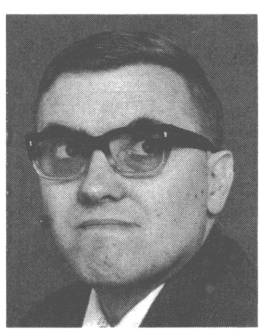
Acknowledgement

The author thanks the editors of *Industrial Quality Control* for permission to reproduce Table V and to quote the example.

References

1. Hewlett-Packard Co., Users' Library, program numbers 03590D, 03591D, 03588D, 03589D.
2. Draper, N., and Smith, H., "Applied Regression Analysis," John Wiley and Sons, New York, 1966, Chapter 10.
3. Smith, H., and Dubey, S. D., *Industrial Quality Control,* Vol. 21, No. 2, pp. 64–70, 1964 (Amer. Soc. for Quality Control, Milwaukee, Wis.).

The author



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Polynomial regression on a pocket calculator

This program for the HP-41C calculator fits a polynomial function to a table of data. The polynomial may then be used for interpolation or mathematical analysis.

Brian W. Clare, *Murdoch University*

☐ Polynomial regression often yields a function that is a good representation of data over a limited range. This program, written for the HP-41C, yields a best-fit polynomial function of a degree specified by the user. At least one 64-register memory module is needed to fit polynomials of degree five or under. With four memory modules (or the 319-register HP-41CV), the program can fit a polynomial up to degree eighteen. A card-reader and printer are convenient to have but are not necessary.

Regression analysis

Finding an equation that represents a table of (x,y) data accurately is a common engineering problem. When the data are the result of an experiment, and contain errors, the best way to do this is by least-squares regression analysis.

Linear regression is the simplest form of regression analysis. Available on most scientific calculators, the technique fits a straight line ($y = ax + b$) to a set of data (x_i,y_i) such that the sum of the squared errors is a minimum. However, data cannot always be approximated by a straight line.

If the form of dependence of y on x is known, then nonlinear regression [*1*] is possible. But there is no way to guarantee convergence of this iterative regression procedure. If the form of dependence is unknown, then y often may be treated as some general function of x—such as a sum of trigonometric terms (Fourier analysis) or a polynomial function. This last case is termed polynomial regression.

How polynomial regression works

Polynomial regression takes a set of N data points (x_i,y_i) and represents it as an nth-degree polynomial:

$$y = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$$

where $a_0, a_1 \cdots a_n$ are constants chosen so that the sum of the squared errors (f) is a minimum:

$$f = \Sigma_i(a_0 + a_1x_i + a_2x_i^2 + \cdots + a_nx_i^n - y_i)^2$$

According to calculus, the function f is a minimum with respect to the choice of coefficients when each of the partial derivatives is zero:

$$\frac{\delta f}{\delta a_0} = \frac{\delta f}{\delta a_1} = \frac{\delta f}{\delta a_2} = \cdots = \frac{\delta f}{\delta a_n} = 0$$

Differentiating f with respect to each of these coefficients and setting the partial derivatives equal to zero gives rise to a system of $(n + 1)$ linear equations in $(n + 1)$ unknowns $(a_0, a_1 \cdots a_n)$:

$$\begin{aligned}
na_0 + a_1\Sigma x_i + a_2\Sigma x_i^2 + \cdots + a_n\Sigma x_i^n &= \Sigma y_i \\
a_0\Sigma x_i + a_1\Sigma x_i^2 + a_2\Sigma x_i^3 + \cdots + a_n\Sigma x_i^{n+1} &= \Sigma x_i y_i \\
a_0\Sigma x_i^2 + a_1\Sigma x_i^3 + a_2\Sigma x_i^4 + \cdots + a_n\Sigma x_i^{n+2} &= \Sigma x_i^2 y_i \\
&\vdots \\
a_0\Sigma x_i^n + a_1\Sigma x_i^{n+1} + a_2\Sigma x_i^{n+2} + \cdots + a_n\Sigma x_i^{2n} &= \Sigma x_i^n y_i
\end{aligned}$$

Since we can calculate the sums and products of the x_i and y_i terms, we can solve this symmetric matrix to find the $a_0, a_1 \cdots a_n$ values. These are the regression coefficients for our nth-degree polynomial.

How the calculator program works

The HP-41C implementation of the polynomial-regression algorithm consists of three parts, which are listed in Table I:

1. Program "POLY."* This 378-byte program handles data input, calculation of sums in the matrix, output of regression coefficients, and calculation of the conditional mean $\bar{y}$ for any given x once the coefficients are known.

2. Subroutine "SYMLIN." This 248-byte routine solves the matrix. It has been described previously [*1*], in greater detail. (See previous article.)

3. Subroutine "FMT." This 17-byte routine formats all numbers displayed and printed by the program. As listed in Table I, "FMT" limits numbers to 5 decimal places and specifies scientific notation for numbers less than or equal to 0.1. If desired, "FMT" can be changed

*Throughout this article, names such as "POLY" that require ALPHA-mode keystrokes will be placed in parentheses. The parentheses are *not* part of the name. Regular keys will be boldfaced; e.g., **R/S**.

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Program "POLY" and subroutines "SYMLIN" and "FMT" occupy 95 storage registers in the HP-41C calculator **Table I**

"POLY"

```
01♦LBL "POLY"
02 CLRG
03 9
04 STO 08
05 "DEGREE?"
06 FIX 0
07 CF 29
08 PROMPT
09 ARCL X
10 AVIEW
11 1
12 +
13 STO 07
14 ADV
15 1
16 STO 06

17♦LBL 05
18 "X"
19 FIX 0
20 CF 29
21 -1
22 RCL 06
23 FS? 00
24 +
25 ARCL X
26 "⊢= "
27 PROMPT
28 XEQ "FMT"
29 SF 29
30 ARCL X
31 AVIEW
32 STO 00
33 "Y"
34 FIX 0
35 CF 29
36 -1
37 RCL 06
38 FS? 00
39 +
40 ARCL X
41 "⊢= "
42 PROMPT
43 SF 29
44 XEQ "FMT"
45 ARCL X
46 AVIEW
47 STO 01
48 XEQ A
49 1
50 FS? 00
51 CHS
52 ST+ 06
53 CF 00
54 ADV
55 GTO 05

56♦LBL A
57 0
58 STO 03
59 RCL 08
60 STO 02
61 1
62 STO 05
63 FS? 00
64 CHS
65 ST+ IND 02

66♦LBL 00
67 1
68 ST+ 03
69 XEQ 09
70 STO 04
71 RCL 03
72 RCL 07
73 2
74 *
75 X=Y?
76 GTO 02
77 RCL 00
78 ST* 05

79♦LBL 01
80 RCL 03
81 RCL 04
82 2
83 *
84 -
85 3
86 +
87 X<=0?
88 GTO 00
89 XEQ 08
90 +
91 STO 02
92 RCL 05
93 FS? 00
94 CHS
95 ST+ IND 02
96 1
97 ST+ 04
98 GTO 01

99♦LBL 02
100 2
101 STO 04

102♦LBL 03
103 XEQ 08
104 STO 02
105 RCL 01
106 FS? 00
107 CHS
108 ST+ IND 02
109 1
110 ST+ 04
111 RCL 00
112 ST* 01
113 RCL 04
114 RCL 07
115 2
116 +
117 X=Y?
118 GTO 04
119 GTO 03

120♦LBL 04
121 RCL 98
122 STO 02
123 RCL IND 02
124 RTN

125♦LBL B
126 "DELETE"
127 AVIEW
128 SF 00
129 GTO 05

130♦LBL 09
131 RCL 03
132 RCL 07
133 -
134 2
135 +
136 1
137 X<=Y?
138 X<>Y
139 RTN

140♦LBL 08
141 RCL 07
142 2
143 *
144 4
145 +
146 RCL 04
147 -
148 RCL 04
149 1
150 -
151 *
152 2
153 /
154 RCL 08
155 +
156 1
157 -
158 RTN

159♦LBL C
160 XEQ "SYMLIN"
161 ADV
162 RCL 08
163 RCL 07
164 RCL 08
165 +
166 1
167 -
168 1 E3
169 /
170 +
171 STO 00

172♦LBL 07
173 "A"
174 FIX 0
175 CF 29
176 ARCL 06
177 "⊢= "
178 SF 29
179 RCL IND 00
180 XEQ "FMT"
181 ARCL X
182 AVIEW
183 FC? 55
184 STOP
185 1
186 ST+ 06
187 ISG 00
188 GTO 07
189 ADV
190 ADV
191 ADV
192 ADV
193 RTN

194♦LBL E
195 ADV
196 "X= "
197 PROMPT
198 XEQ "FMT"
199 SF 29
200 ARCL X
201 AVIEW
202 ENTER↑
203 ENTER↑
204 ENTER↑
205 RCL 08
206 RCL 07
207 +
208 RCL 08
209 1 E3
210 /
211 +
212 1
213 -
214 STO 00
215 CLX

216♦LBL 06
217 RCL IND 00
218 +
219 *
220 DSE 00
221 GTO 06
222 RCL IND 00
223 +
224 "YBAR= "
225 XEQ "FMT"
226 ARCL X
227 AVIEW
228 FC? 55
229 STOP
230 GTO E
231 END
```

"SYMLIN"

```
01♦LBL "SYMLIN"
02 RCL 07
03 STO 00
04 RCL 08
05 STO 01

06♦LBL C
07 RCL 01
08 STO 06
09 1
10 STO 02

11♦LBL 01
12 RCL 06
13 STO 03
14 ISG 03

15♦LBL 09
16 RCL IND 03
17 RCL IND 01
18 /
19 STO 05
20 XEQ 08
21 STO 04
22 1
23 ST+ 02
24 XEQ 08
25 1
26 -
27 1 E3
28 /
29 ST+ 04

30♦LBL 00
31 RCL IND 03
32 RCL 05
33 *
34 ST- IND 04
35 ISG 03

36♦LBL 09
37 ISG 04
38 GTO 00
39 1
40 ST+ 06
41 RCL 06
42 RCL 01
43 -
44 RCL 00
45 1
46 -
47 X≠Y?
48 GTO 01
49 RCL 00
50 1
51 +
52 ST+ 01
53 1
54 ST- 00
55 RCL 00
56 1
57 X≠Y?
58 GTO C
59 RCL 08
60 STO 01
61 RCL 07
62 STO 00
63 STO 02
64 1
65 -
66 STO 06
67 1
68 STO 05
69 XEQ 08
70 1
71 -
72 STO 03
73 RCL IND 03
74 DSE 03
75 RCL IND 03
```

(Continued) Table I

```
 76 /
 77 ISG 03

 78♦LBL 09
 79 STO IND 03
 80 STO 04

 81♦LBL A
 82 RCL 06
 83 STO 02

 84♦LBL 03
 85 XEQ 08
 86 1
 87 -
 88 RCL 05
 89 -
 90 STO 03
 91 RCL 04
 92 ST* IND 03
 93 DSE 02
 94 GTO 03
 95 DSE 06

 96♦LBL 09
 97 RCL 06
 98 STO 02
 99 XEQ 08
100 STO 03
101 1
102 ST+ 02
103 XEQ 08
104 2
105 -
106 1 E3
107 /
108 ST+ 03
109 RCL IND 03
110 STO 04
111 1
112 ST+ 03

113♦LBL 05
114 RCL IND 03
115 ISG 03
116 GTO 07
117 GTO 06

118♦LBL 07
119 ST+ IND 03
120 GTO 05

121♦LBL 06
122 ST- IND 03
123 RCL 04
124 ST/ IND 03
125 RCL IND 03
126 STO 04
127 RCL 06
128 X=0?
129 GTO D
130 1
131 ST+ 05
132 GTO A

133♦LBL D
134 RCL 00
135 STO 02
136 RCL 01
137 +
138 1
139 -
140 STO 04

141♦LBL 11
142 XEQ 08
143 1
144 -
145 STO 03
146 RCL IND 03
147 STO IND 04
148 DSE 04

149♦LBL 09
150 DSE 02
151 GTO 11
152 RTN

153♦LBL 08
154 RCL 00
155 1.5
156 +
157 RCL 02
158 2
159 /
160 -
161 RCL 02
162 *
163 RCL 01
164 +
165 RTN
166 END
```

"FMT"

```
01♦LBL "FMT"
02 .1
03 X<>Y
04 X>Y?
05 GTO 00
06 SCI 5
07 RTN

08♦LBL 00
09 2
10 X<>Y
11 X>Y?
12 GTO 01
13 FIX 5
14 RTN

15♦LBL 01
16 FIX 5
17 RTN
18 .END.
```

Notes:
"POLY" is 378 bytes.
"SYMLIN" is 248 bytes.
"FMT" is 17 bytes.
"FMT" sets the output and display format.
The alternative "FMT" listed below will display all numbers in 5-decimal scientific notation:

```
01♦LBL "FMT"
02 SCI 5
03 .END.
```

to fit the needs of a particular problem. Changing it to the alternative form also listed in Table I will assure that any number can be displayed without loss of precision—though the display may be difficult to read because of the exponents.

The program allocates the storage as follows: Registers 00 and 01 hold the most recent x and y values; Registers 02, 07 and 08 are used; Registers from 09 onward hold the matrix. Since the matrix is symmetric, only half is stored.

Using the program

Table II lists user instructions for the program. Several points that should be noted are:

1. The program should be loaded and run in the USER mode. This enables one to press single keys during execution rather than giving **XEQ** commands (e.g., pressing the **B** key rather than **XEQ** "B").

2. One must allocate registers to data storage. The program requires a total of 95 registers. This means that an HP-41C calculator equipped with m 64-register memory modules has $(64m - 32)$ registers available for allocation. The HP-41CV has 224 registers available. A polynomial of degree n needs $(0.5n^2 + 2.5n + 11)$ registers, at a minimum.

3. The program requires that one decide the degree (n) of polynomial. This should not be greater than (N − 1), where N is the number of data points, nor less

User instructions for HP-41C program **Table II**

Step	Entries	Display/Prompting
1. Allocate storage	**XEQ** "SIZE" (No. of registers)	SIZE – – –
2. Set USER mode	**USER**	
3. Load or read program		
4. Enter degree (n) and (x,y) data	**XEQ** "POLY"	DEGREE?
	(Degree) **R/S**	X1=
	(x_1) **R/S**	Y1=
	(y_1) **R/S**	X2= (after execution delay)
	(x_2) **R/S**	Y2=
	(etc. through y_N)	
5. To delete a point*	**B**	DELETE
		X_j =(where y_j was last point entered)
	(x_j) **R/S**	Y_j =
	(y_j) **R/S**	X_j = (enter next or corrected point)
6. Calculate regression coefficients*	**C**	A0= (a_0)
	R/S	A1= (a_1)
	R/S	A2= (a_2)
	(etc. through a_n)	
7. Calculate conditional means*	**E**	X=
	(x) **R/S**	YBAR = (y value for given x)
	(x) **R/S**	YBAR = (etc.)
8. To enter new data	Return to Step 4	

*If calculator is not in USER mode, press **XEQ** "B" (or "C," etc.) rather than the **B** key.

Example data: Specific heat of water — **Table III**

T,°C	c_p	T,°C	c_p
0	1.00762	55	0.99919
5	1.00392	60	0.99967
10	1.00153	65	1.00024
15	1.00000	70	1.00091
20	0.99907	75	1.00167
25	0.99852	80	1.00253
30	0.99826	85	1.00351
35	0.99818	90	1.00461
40	0.99828	95	1.00586
45	0.99849	100	1.00721
50	0.99878		

Source: Ref. 2. Used with permission of John Wiley & Sons.

than 1, which would be a linear regression. Note that one memory module allows n to be no greater than 5; n can be as high as 18 with four memory modules.

4. During data entry, the execution time after entry of each y value depends on the degree of the polynomial: about 20 s for degree 2; 50 s for degree 4; 80 s for degree 6; 120 s for degree 8; up to about 6 min for degree 18. This should be considered in choosing the degree. Note that execution time may depend on the particular calculator.

5. Subroutine "SYMLIN" destroys the matrix when it calculates the regression coefficients. Therefore, points cannot be added or deleted after **C** is executed.

6. If a printer is used (MAN mode), all the data and coefficients are printed out.

Example results show good fit of sixth-degree polynomial — **Table IV**

Regression coefficients	Values of *y* per regression equation		
A0= 1.00760	X= 0.00000E0 YBAR= 1.00760	X= 35.00000 YBAR= 0.99821	X= 70.00000 YBAR= 1.00091
A1= -8.79449E-4			
A2= 3.33998E-5			
A3= -6.87661E-7	X= 5.00000 YBAR= 1.00396	X= 40.00000 YBAR= 0.99829	X= 75.00000 YBAR= 1.00168
A4= 8.31908E-9			
A5= -5.29596E-11			
A6= 1.38922E-13	X= 10.00000 YBAR= 1.00154	X= 45.00000 YBAR= 0.99849	X= 80.00000 YBAR= 1.00255
	X= 15.00000 YBAR= 0.99999	X= 50.00000 YBAR= 0.99879	X= 85.00000 YBAR= 1.00352
	X= 20.00000 YBAR= 0.99904	X= 55.00000 YBAR= 0.99917	X= 90.00000 YBAR= 1.00461
	X= 25.00000 YBAR= 0.99851	X= 60.00000 YBAR= 0.99965	X= 95.00000 YBAR= 1.00583
	X= 30.00000 YBAR= 0.99826	X= 65.00000 YBAR= 1.00023	X= 100.00000 YBAR= 1.00723

Example

McCracken and Dorn [2] list data for the specific heat of water at various temperatures, and show a third-degree polynomial approximation of that data. Their data are listed in Table III. Since their polynomial appeared not to fit well, let us try a sixth-degree polynomial approximation.

Table IV shows the actual output of the program. The regression coefficients a_0–a_6 are listed, and the regression equation is therefore:

$$y = 1.00760 - 8.79449 \times 10^{-4}x + 3.33998 \times 10^{-5}x^2 - 6.87661 \times 10^{-7}x^3 + 8.31908 \times 10^{-9}x^4 - 5.29596 \times 10^{-11}x^5 + 1.38922 \times 10^{-13}x^6$$

Table IV also lists the conditional means (YBAR) predicted by the regression equation for each temperature (X) in the original data. Comparing these calculated values of specific heat with the actual data, one can see that the fit is very good—a maximum deviation of 0.00004, or less than 0.005%. Of course, the y data in this example fell into a very narrow range (1.003 ± 0.005).

Cautions

The system of linear equations generated by polynomial regression can be ill-conditioned—leading to smooth curves that fit poorly—if the degree of the polynomial is large and especially if the y values cover a wide range. This means inaccurate results, and can be avoided only by using orthogonal polynomials instead of powers of x as the regression functions.

The regression equation begins to reproduce the errors of measurement as well as the true trend when the degree of the polynomial approaches the number of data points. When $n = (N - 1)$, the polynomial fits perfectly but is not a satisfactory representation of the data. The true best fit is given by the polynomial function where $\Sigma(\bar{y}_i - y_i)^2/(N - n - 1)$ shows no further significant decrease ($\bar{y}$ is the y value for a given x predicted by the regression equation). To get this best fit, one must try several degrees of polynomial and calculate conditional means and squared error each time.

As a final caution, be aware that extrapolation with polynomials is always dangerous and becomes more so as the degree of the polynomial increases. It is best to use the regression equation only within the limits of the original data.

Conditionals, such as X = Y?, X = O?, etc., should be entered as commands; they should not be inserted as ALPHA strings (i.e., enclosed in quotation marks).

For TI users

The TI version for calculating the best-fit polynomial function for a given set of data closely follows the HP program. However, the TI version is limited to a maximum of a fourth-degree equation. Tables V and VI present the listings of the TI programs. User instructions are offered in Table VII.

Listing for TI version—program 1 **Table V**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	063	43	RCL	126	22	INV	189	75	-	252	42	STO
001	11	A	064	16	16	127	44	SUM	190	43	RCL	253	14	14
002	87	IFF	065	44	SUM	128	13	13	191	07	07	254	43	RCL
003	01	01	066	10	10	129	43	RCL	192	55	÷	255	05	05
004	22	INV	067	65	×	130	15	15	193	43	RCL	256	55	÷
005	47	CMS	068	43	RCL	131	45	Y^x	194	05	05	257	43	RCL
006	86	STF	069	15	15	132	05	5	195	95	=	258	03	03
007	01	01	070	95	=	133	95	=	196	42	STO	259	75	-
008	42	STO	071	44	SUM	134	22	INV	197	24	24	260	43	RCL
009	00	00	072	11	11	135	44	SUM	198	43	RCL	261	06	06
010	91	R/S	073	65	×	136	06	06	199	07	07	262	55	÷
011	76	LBL	074	43	RCL	137	65	×	200	55	÷	263	43	RCL
012	22	INV	075	15	15	138	43	RCL	201	43	RCL	264	04	04
013	42	STO	076	95	=	139	15	15	202	04	04	265	95	=
014	16	16	077	44	SUM	140	95	=	203	75	-	266	42	STO
015	32	X:T	078	12	12	141	22	INV	204	43	RCL	267	18	18
016	42	STO	079	65	×	142	44	SUM	205	08	08	268	43	RCL
017	15	15	080	43	RCL	143	07	07	206	55	÷	269	06	06
018	99	PRT	081	15	15	144	65	×	207	43	RCL	270	55	÷
019	44	SUM	082	33	X^2	145	43	RCL	208	05	05	271	43	RCL
020	02	02	083	95	=	146	15	15	209	95	=	272	03	03
021	33	X^2	084	44	SUM	147	95	=	210	42	STO	273	75	-
022	44	SUM	085	14	14	148	22	INV	211	25	25	274	43	RCL
023	03	03	086	69	OP	149	44	SUM	212	43	RCL	275	07	07
024	33	X^2	087	21	21	150	08	08	213	08	08	276	55	÷
025	44	SUM	088	98	ADV	151	43	RCL	214	55	÷	277	43	RCL
026	05	05	089	91	R/S	152	16	16	215	43	RCL	278	04	04
027	33	X^2	090	76	LBL	153	22	INV	216	04	04	279	95	=
028	44	SUM	091	12	B	154	44	SUM	217	75	-	280	42	STO
029	09	09	092	42	STO	155	10	10	218	43	RCL	281	19	19
030	43	RCL	093	16	16	156	65	×	219	09	09	282	43	RCL
031	15	15	094	32	X:T	157	43	RCL	220	55	÷	283	07	07
032	45	Y^x	095	42	STO	158	15	15	221	43	RCL	284	55	÷
033	03	3	096	15	15	159	95	=	222	05	05	285	43	RCL
034	95	=	097	99	PRT	160	22	INV	223	95	=	286	03	03
035	44	SUM	098	22	INV	161	44	SUM	224	42	STO	287	75	-
036	04	04	099	44	SUM	162	11	11	225	26	26	288	43	RCL
037	65	×	100	02	02	163	65	×	226	43	RCL	289	08	08
038	43	RCL	101	33	X^2	164	43	RCL	227	13	13	290	55	÷
039	16	16	102	22	INV	165	15	15	228	55	÷	291	43	RCL
040	99	PRT	103	44	SUM	166	95	=	229	43	RCL	292	04	04
041	95	=	104	03	03	167	22	INV	230	04	04	293	95	=
042	44	SUM	105	33	X^2	168	44	SUM	231	75	-	294	42	STO
043	13	13	106	22	INV	169	12	12	232	43	RCL	295	20	20
044	43	RCL	107	44	SUM	170	65	×	233	14	14	296	43	RCL
045	15	15	108	05	05	171	43	RCL	234	55	÷	297	12	12
046	45	Y^x	109	33	X^2	172	15	15	235	43	RCL	298	55	÷
047	05	5	110	22	INV	173	33	X^2	236	05	05	299	43	RCL
048	95	=	111	44	SUM	174	95	=	237	95	=	300	03	03
049	44	SUM	112	09	09	175	22	INV	238	42	STO	301	75	-
050	06	06	113	43	RCL	176	44	SUM	239	09	09	302	43	RCL
051	65	×	114	15	15	177	14	14	240	43	RCL	303	13	13
052	43	RCL	115	45	Y^x	178	69	OP	241	05	05	304	55	÷
053	15	15	116	03	3	179	31	31	242	55	÷	305	43	RCL
054	95	=	117	95	=	180	98	ADV	243	43	RCL	306	04	04
055	44	SUM	118	22	INV	181	91	R/S	244	04	04	307	95	=
056	07	07	119	44	SUM	182	76	LBL	245	75	-	308	42	STO
057	65	×	120	04	04	183	13	C	246	43	RCL	309	08	08
058	43	RCL	121	65	×	184	43	RCL	247	06	06	310	43	RCL
059	15	15	122	43	RCL	185	06	06	248	55	÷	311	04	04
060	95	=	123	16	16	186	55	÷	249	43	RCL	312	55	÷
061	44	SUM	124	99	PRT	187	43	RCL	250	05	05	313	43	RCL
062	08	08	125	95	=	188	04	04	251	95	=	314	03	03

(Continued) Table V

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
315	75	-	348	03	03	381	03	03	414	43	RCL	447	95	=
316	43	RCL	349	95	=	382	55	÷	415	05	05	448	42	STO
317	05	05	350	42	STO	383	43	RCL	416	55	÷	449	06	06
318	55	÷	351	22	22	384	02	02	417	43	RCL	450	43	RCL
319	43	RCL	352	43	RCL	385	75	-	418	02	02	451	02	02
320	04	04	353	06	06	386	43	RCL	419	95	=	452	55	÷
321	95	=	354	55	÷	387	04	04	420	42	STO	453	43	RCL
322	42	STO	355	43	RCL	388	55	÷	421	16	16	454	01	01
323	13	13	356	02	02	389	43	RCL	422	43	RCL	455	75	-
324	43	RCL	357	75	-	390	03	03	423	05	05	456	43	RCL
325	04	04	358	43	RCL	391	95	=	424	55	÷	457	03	03
326	55	÷	359	07	07	392	42	STO	425	43	RCL	458	55	÷
327	43	RCL	360	55	÷	393	12	12	426	01	01	459	43	RCL
328	02	02	361	43	RCL	394	43	RCL	427	75	-	460	02	02
329	75	-	362	03	03	395	03	03	428	43	RCL	461	95	=
330	43	RCL	363	95	=	396	55	÷	429	06	06	462	42	STO
331	05	05	364	42	STO	397	43	RCL	430	55	÷	463	11	11
332	55	÷	365	23	23	398	01	01	431	43	RCL	464	43	RCL
333	43	RCL	366	43	RCL	399	75	-	432	02	02	465	08	08
334	03	03	367	11	11	400	43	RCL	433	95	=	466	55	÷
335	95	=	368	55	÷	401	04	04	434	42	STO	467	43	RCL
336	42	STO	369	43	RCL	402	55	÷	435	17	17	468	13	13
337	21	21	370	02	02	403	43	RCL	436	43	RCL	469	75	-
338	43	RCL	371	75	-	404	02	02	437	10	10	470	43	RCL
339	05	05	372	43	RCL	405	95	=	438	55	÷	471	09	09
340	55	÷	373	12	12	406	42	STO	439	43	RCL	472	55	÷
341	43	RCL	374	55	÷	407	15	15	440	01	01	473	43	RCL
342	02	02	375	43	RCL	408	43	RCL	441	75	-	474	14	14
343	75	-	376	03	03	409	04	04	442	43	RCL	475	95	=
344	43	RCL	377	95	=	410	55	÷	443	11	11	476	42	STO
345	06	06	378	42	STO	411	43	RCL	444	55	÷	477	09	09
346	55	÷	379	07	07	412	01	01	445	43	RCL	478	91	R/S
347	43	RCL	380	43	RCL	413	75	-	446	02	02			

Listing for TI version—program 2 **Table VI**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	022	43	RCL	044	55	÷	066	55	÷	088	13	13
001	13	C	023	06	06	045	43	RCL	067	43	RCL	089	95	=
002	43	RCL	024	55	÷	046	14	14	068	13	13	090	42	STO
003	07	07	025	43	RCL	047	95	=	069	75	-	091	18	18
004	55	÷	026	11	11	048	42	STO	070	43	RCL	092	43	RCL
005	43	RCL	027	75	-	049	24	24	071	26	26	093	22	22
006	12	12	028	43	RCL	050	43	RCL	072	55	÷	094	55	÷
007	75	-	029	07	07	051	19	19	073	43	RCL	095	43	RCL
008	43	RCL	030	55	÷	052	55	÷	074	14	14	096	12	12
009	08	08	031	43	RCL	053	43	RCL	075	95	=	097	75	-
010	55	÷	032	12	12	054	13	13	076	42	STO	098	43	RCL
011	43	RCL	033	95	=	055	75	-	077	26	26	099	19	19
012	13	13	034	42	STO	056	43	RCL	078	43	RCL	100	55	÷
013	95	=	035	07	07	057	25	25	079	21	21	101	43	RCL
014	42	STO	036	43	RCL	058	55	÷	080	55	÷	102	13	13
015	08	08	037	18	18	059	43	RCL	081	43	RCL	103	95	=
016	43	RCL	038	55	÷	060	14	14	082	12	12	104	42	STO
017	00	00	039	43	RCL	061	95	=	083	75	-	105	19	19
018	32	X:T	040	13	13	062	42	STO	084	43	RCL	106	43	RCL
019	01	1	041	75	-	063	25	25	085	18	18	107	23	23
020	67	EQ	042	43	RCL	064	43	RCL	086	55	÷	108	55	÷
021	23	LNX	043	24	24	065	20	20	087	43	RCL	109	43	RCL

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
110	12	12	176	95	=	242	19	19	308	43	RCL	374	75	-
111	75	-	177	42	STO	243	55	÷	309	07	07	375	43	RCL
112	43	RCL	178	09	09	244	43	RCL	310	75	-	376	33	33
113	20	20	179	43	RCL	245	18	18	311	43	RCL	377	65	×
114	55	÷	180	07	07	246	95	=	312	33	33	378	43	RCL
115	43	RCL	181	55	÷	247	42	STO	313	65	×	379	04	04
116	13	13	182	43	RCL	248	18	18	314	43	RCL	380	75	-
117	95	=	183	14	14	249	03	3	315	13	13	381	43	RCL
118	42	STO	184	75	-	250	67	EQ	316	75	-	382	34	34
119	20	20	185	43	RCL	251	25	CLR	317	43	RCL	383	65	×
120	43	RCL	186	08	08	252	43	RCL	318	34	34	384	43	RCL
121	15	15	187	55	÷	253	08	08	319	65	×	385	05	05
122	55	÷	188	43	RCL	254	55	÷	320	43	RCL	386	95	=
123	43	RCL	189	18	18	255	43	RCL	321	12	12	387	55	÷
124	11	11	190	95	=	256	18	18	322	95	=	388	43	RCL
125	75	-	191	42	STO	257	75	-	323	55	÷	389	01	01
126	43	RCL	192	08	08	258	43	RCL	324	43	RCL	390	95	=
127	21	21	193	43	RCL	259	09	09	325	14	14	391	42	STO
128	55	÷	194	20	20	260	55	÷	326	95	=	392	30	30
129	43	RCL	195	55	÷	261	43	RCL	327	42	STO	393	99	PRT
130	12	12	196	43	RCL	262	25	25	328	32	32	394	98	ADV
131	95	=	197	18	18	263	95	=	329	99	PRT	395	22	INV
132	42	STO	198	75	-	264	42	STO	330	76	LBL	396	86	STF
133	14	14	199	43	RCL	265	09	09	331	23	LNX	397	01	01
134	43	RCL	200	26	26	266	43	RCL	332	43	RCL	398	91	R/S
135	16	16	201	55	÷	267	20	20	333	06	06	399	76	LBL
136	55	÷	202	43	RCL	268	55	÷	334	75	-	400	15	E
137	43	RCL	203	24	24	269	43	RCL	335	43	RCL	401	42	STO
138	11	11	204	95	=	270	18	18	336	32	32	402	15	15
139	75	-	205	42	STO	271	75	-	337	65	×	403	65	×
140	43	RCL	206	26	26	272	43	RCL	338	43	RCL	404	43	RCL
141	22	22	207	43	RCL	273	26	26	339	15	15	405	31	31
142	55	÷	208	19	19	274	55	÷	340	75	-	406	85	+
143	43	RCL	209	55	÷	275	43	RCL	341	43	RCL	407	43	RCL
144	12	12	210	43	RCL	276	25	25	342	33	33	408	30	30
145	95	=	211	18	18	277	95	=	343	65	×	409	85	+
146	42	STO	212	75	-	278	42	STO	344	43	RCL	410	43	RCL
147	13	13	213	43	RCL	279	25	25	345	16	16	411	15	15
148	43	RCL	214	25	25	280	35	1/X	346	75	-	412	33	X^2
149	17	17	215	55	÷	281	65	×	347	43	RCL	413	65	×
150	55	÷	216	43	RCL	282	43	RCL	348	34	34	414	43	RCL
151	43	RCL	217	24	24	283	09	09	349	65	×	415	32	32
152	11	11	218	95	=	284	95	=	350	43	RCL	416	85	+
153	75	-	219	42	STO	285	42	STO	351	17	17	417	53	(
154	43	RCL	220	25	25	286	34	34	352	95	=	418	43	RCL
155	23	23	221	43	RCL	287	99	PRT	353	55	÷	419	15	15
156	55	÷	222	12	12	288	76	LBL	354	43	RCL	420	45	Y^X
157	43	RCL	223	55	÷	289	25	CLR	355	11	11	421	03	3
158	12	12	224	43	RCL	290	43	RCL	356	95	=	422	54	)
159	95	=	225	14	14	291	08	08	357	42	STO	423	65	×
160	42	STO	226	75	-	292	75	-	358	31	31	424	43	RCL
161	12	12	227	43	RCL	293	43	RCL	359	99	PRT	425	33	33
162	02	2	228	20	20	294	34	34	360	43	RCL	426	85	+
163	67	EQ	229	55	÷	295	65	×	361	10	10	427	53	(
164	24	CE	230	43	RCL	296	43	RCL	362	75	-	428	43	RCL
165	43	RCL	231	18	18	297	20	20	363	43	RCL	429	15	15
166	08	08	232	95	=	298	95	=	364	31	31	430	45	Y^X
167	55	÷	233	42	STO	299	55	÷	365	65	×	431	04	4
168	43	RCL	234	20	20	300	43	RCL	366	43	RCL	432	54	)
169	18	18	235	43	RCL	301	18	18	367	02	02	433	65	×
170	75	-	236	13	13	302	95	=	368	75	-	434	43	RCL
171	43	RCL	237	55	÷	303	42	STO	369	43	RCL	435	34	34
172	09	09	238	43	RCL	304	33	33	370	32	32	436	95	=
173	55	÷	239	14	14	305	99	PRT	371	65	×	437	99	PRT
174	43	RCL	240	75	-	306	76	LBL	372	43	RCL	438	91	R/S
175	24	24	241	43	RCL	307	24	CE	373	03	03			

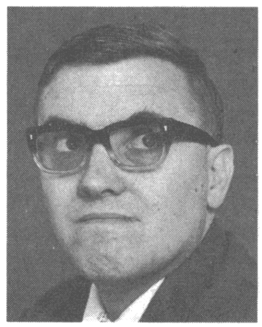
User instructions for the TI version **Table VII**

Step	Input	Key	Output
1. Load program 1			
2. Enter degree (n)	(Degree) (1 to 4)	A	
3. Input data:	x_i	x ⇌ t	
	y_i	A	
	Repeat until all data are entered.		
	(To delete an erroneous pair of values:		
	x_i	x ⇌ t	
	y_i	B	
4. When all data are entered		C	Starts calculation
5. When calculation stops, load program 2			
6. After loading program 2		C	Completes calculation
7. Calculate regression coefficients*			a_n, a_{n-1}, a_{n-2}, etc.
8. Calculate conditional means	x	E	$\bar{y}$ (YBAR, y value for a given x)

*Output is the regression coefficients, starting with the highest degree and ending with a_0. For instance, for a third-degree calculation: $y = a_0 + a_1x + a_2x^2 + a_3x^3$, the output is a_3, a_2, a_1, a_0.

References

1. Clare, B. W., Nonlinear regression on a pocket calculator, *Chem. Eng.*, Aug. 23, 1982, pp. 83–89.
2. McCracken, D. D., and Dorn, W. S., "Numerical Methods with FORTRAN IV Case Studies," John Wiley & Sons, New York, 1972, Fig. 7.9 and Table 7.5. Used with permission.



The author

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Curve fitting via orthogonal polynomials

In fitting a curve to experimental data, it may be desirable to use polynomials of increasing degree until the necessary fit is achieved. Employing orthogonal polynomials has several advantages.

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☐ The first thing to do in fitting a curve to experimental data is to choose a suitable type of function. Sometimes this is easy, the mathematical form of the function being known. Vapor-pressure/temperature data, for example, can be fitted to an equation of the form:

$$P = A\, e^{-B/T}$$

with a reasonable degree of accuracy, and this can be converted to a linear regression problem by taking logarithms of both sides.

In other cases, a nonlinear equation may be appropriate, and fitting this requires an iterative method [*1*].

If no functional relationship is known or, in some cases, if a nonlinear equation is known, it may be appropriate to use polynomials of increasing degree until the desired fit is achieved. Polynomials are very flexible, and can be fitted to most continuous functions. A procedure for fitting polynomials by solving the normal equations has already been described [*2*]. It was pointed out in that article, however, that poor results can be obtained when the degree of the polynomial is large, or when the dependent variable covers a wide range.

This is because the normal equations in this case become extremely ill-conditioned, meaning that a small error in the data (or, as in this case, in the intermediate results) makes a large difference in the final result.

If, instead of powers of x, a set of orthogonal polynomials are used, the solution of the normal equations can be avoided. Thus, instead of the relationship:

$$y = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n \quad (1)$$

we fit the equation:

$$y = b_0P_0(x) + b_1P_1(x) + \cdots + b_iP_i(x) + \cdots + b_nP_n(x) \quad (2)$$

where $P_i(x)$ is an ith-degree polynomial in x, and $P_j(x)$ is a jth-degree polynomial in x.

These two polynomials are said to be orthogonal if the sum:

$$\sum_{0}^{n} P_i(x)P_j(x)$$

is zero when $i \neq j$, and is non-zero when $i = j$. The summation extends over all points.

The use of such polynomials has several advantages:

1. The solution of the normal equations is avoided, and the problem is not ill-conditioned. A high-degree polynomial can be fitted without any problems.

2. The amount of calculation involved is greatly reduced, so the method is much faster.

3. Normally, if a least-squares polynomial of degree n is fitted to data, a truncated version of degree $m(m \leq n)$ will not be a least-squares fit. However, with this method, the program stores a sequence of orthogonal polynomials that remain least-square fits, even when truncated. Hence the user can select any degree (m) of polynomial, up to the value n, which provides a satisfactory fit. This may be done without reentry of data. The method of determining the quality of fit is discussed later.

However, the advantages are obtained at a price—the values of the independent variable must be equally spaced.

The method of fitting these orthogonal polynomials is given in Ref. 3 and 4, and will not be reproduced here. However, for further reference, it may be useful to know that the term Gram polynomials refers to a particular set of polynomials that are orthogonal on discrete, equally-spaced points. These are sometimes called Chebychev polynomials, but this name is also used for other types of orthogonal polynomials.

Use of the HP41C program

The program is given in Table I. To use it, the program must be loaded into memory with a formatting subroutine under label FMT: (PGM) LBL 'FMT' FIX 4 RTN (PGM). This subroutine determines the format of all data and results, and can, if desired, be more complex than this simple, four-decimal-point output.

The program calls for the operator to select a degree, m, of polynomial that might fit the data sufficiently well, where $m \leq n$. For each degree, m, that is tested, we obtain a set of coefficients, a, and a set of conditional means, y bar. If these conditional means are sufficiently close to the actual y values, the polynomial may be

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Program fits curves to a high degree of accuracy via orthogonal polynomials **Table I**

```
01♦LBL "PO  "
02 CLRG
03 "HOW MANY POINTS"
04 "⊢ ?"
05 PROMPT
06 CLA
07 FIX 0
08 CF 29
09 ARCL X
10 "⊢ POINTS"
11 AVIEW
12 1
13 -
14 STO 09
15 "MAXIMUM DEGREE "
16 "⊢? "
17 PROMPT
18 STO 04
19 ARCL X
20 AVIEW
21 ADV
22 "INITIAL X? "
23 PROMPT
24 XEQ "FMT"
25 STO 08
26 ARCL X
27 AVIEW
28 "FINAL X? "
29 PROMPT
30 XEQ "FMT"
31 ARCL X
32 AVIEW
33 STO 09
34 RCL 08
35 +
36 RCL 09
37 RCL 08
38 -
39 /
40 X<> 09
41 RCL 08
42 -
43 2
44 X<>Y
45 /
46 CHS
47 STO 08
48 ADV
49 0
50♦LBL 00
51 RCL 00
52 1
53 +
54 RCL 10
55 X=Y?
56 GTO 02
57 "Y"
58 FIX 0
59 ARCL X
60 "⊢= "
61 PROMPT
62 XEQ "FMT"
63 ARCL X
64 AVIEW
65♦LBL A
66 STO 06
67 ST+ 11
68 RCL 10
69 2
70 CHS
71 *
72 RCL 00
73 /
74 1
75 STO 02
76 +
77 STO 03
78 RCL 06
79 *
80 ST+ 12
81 13
82 STO 07
83 1
84 STO 01
85♦LBL 01
86 RCL 01
87 RCL 04
88 X=Y?
89 GTO 09
90 RCL 00
91 RCL 01
92 +
93 1
94 +
95 RCL 01
96 *
97 RCL 02
98 *
99 CHS
100 RCL 00
101 RCL 10
102 2
103 *
104 -
105 RCL 01
106 2
107 *
108 1
109 +
110 *
111 RCL 03
112 *
113 +
114 RCL 01
115 1
116 +
117 /
118 RCL 00
119 RCL 01
120 -
121 /
122 RCL 03
123 STO 02
124 RDN
125 STO 03
126 RCL 03
127 RCL 06
128 *
129 ST+ IND 07
130 1
131 ST+ 07
132 ST+ 01
133 GTO 01
134♦LBL 09
135 1
136 ST+ 10
137 GTO 00
138♦LBL 03
139 RCL 00
140 RCL 01
141 X=0?
142 GTO 13
143 +
144 2
145 +
146 STO 02
147 1
148 STO 03
149♦LBL 10
150 1
151 ST- 02
152 RCL 02
153 ST* 03
154 RCL 02
155 RCL 00
156 1
157 +
158 X≠Y?
159 GTO 10
160 RCL 00
161 RCL 01
162 -
163 STO 02
164♦LBL 11
165 1
166 ST- 02
167 RCL 02
168 ST/ 03
169 RCL 02
170 RCL 00
171 X≠Y?
172 GTO 11
173 RCL 03
174 RCL 01
175 2
176 *
177 1
178 +
179 /
180 RTN
181♦LBL 13
182 RCL 00
183 1
184 +
185 RTN
186♦LBL 02
187 11
188 STO 07
189 0
190 STO 01
191♦LBL 12
192 XEQ 03
193 ST/ IND 07
194 1
195 ST+ 01
196 ST+ 07
197 RCL 01
198 RCL 04
199 1
200 +
201 X≠Y?
202 GTO 12
203 1
204 ST+ 04
205♦LBL B
206 ADV
207 "DEGREE? "
208 FIX 0
209 PROMPT
210 ARCL X
211 AVIEW
212 STO 05
213 12
214 RCL 04
215 +
216 ENTER↑
217 ENTER↑
218 RCL 04
219 2
220 *
221 +
222 2
223 +
224 1 E3
225 /
226 +
227 STO 07
228 0
229♦LBL 04
230 STO IND 07
231 ISG 07
232 GTO 04
233 11
234 STO 02
235 RCL 04
236 +
237 1
238 +
239 STO 07
240 RCL 04
241 +
242 1
243 +
244 STO 03
245 1
246 STO IND 07
247 ISG 07
248♦LBL 07
249 STO IND 07
250 RCL IND 02
251 STO IND 03
252 1
253 ST+ 02
254 ST+ 03
255 RCL IND 02
256 STO IND 03
257 1
258 STO 01
259 CF 00
260♦LBL 05
261 1
262 ST+ 02
263 11
264 RCL 04
265 +
266 1
267 +
268 1
269 X<>Y
270 FS? 00
271 +
272 STO 07
273 RCL 00
274 RCL 01
275 +
276 1
277 +
278 RCL 01
279 *
280 RCL 00
281 RCL 01
282 -
283 /
284 RCL 01
285 1
286 +
287 /
288 CHS
289 STO 06
290♦LBL 06
291 RCL IND 07
292 X=0?
293 GTO 08
294 RCL 06
295 RCL IND 07
296 *
297 STO IND 07
298 2
299 ST+ 07
300 GTO 06
301♦LBL 08
302 11
303 RCL 04
304 +
305 1
306 X<>Y
307 FC? 00
308 +
309 STO 07
310 RCL 01
311 2
312 *
313 1
314 +
315 RCL 00
316 *
317 RCL 01
318 1
319 +
320 /
321 RCL 00
322 RCL 01
323 -
324 /
325 STO 06
326♦LBL 14
327 ISG 07
328♦LBL 07
329 RCL 06
330 RCL IND 07
331 X=0?
332 GTO 23
333 *
334 ISG 07
335♦LBL 07
336 ST+ IND 07
337 GTO 14
338♦LBL 23
339 1
340 ST+ 01
341 12
342 ENTER↑
```

(Continued) Table I

```
343 1                382 SF 00            421 *                460 STO 07           499 GTO 35           538 AVIEW
344 X<>Y             383 RTN              422 ST+ 06           461 1                500 ADV              539 FC? 55
345 FS? 02           384♦LBL 25           423 RCL 09           462 STO 06           501 STOP             540 STOP
346 +                385 CF 00            424 ST* 10           463♦LBL 40           502♦LBL C            541 GTO C
347 RCL 04           386 RTN              425 ISG 03           464 RCL 06           503 ADV              542♦LBL 31
348 +                387♦LBL 45           426♦LBL 07           465 ST* IND 07       504 "X= "            543 RCL 03
349 STO 07           388 RCL 04           427 ISG 01           466 RCL 08           505 PROMPT           544 X=0?
350 RCL 04           389 2                428 GTO 32           467 ST* 06           506 XEQ "FMT"        545 GTO 29
351 +                390 *                429 1                468 ISG 07           507 ARCL X           546 RCL 02
352 1                391 12               430 ST+ 02           469 GTO 40           508 AVIEW            547 X=0?
353 +                392 +                431 RCL 02           470 ADV              509 STO 01           548 GTO 29
354 STO 03           393 ENTER↑           432 STO 03           471 RCL 04           510 RCL 04           549 X=Y?
355 XEQ 24           394 ENTER↑           433 RCL 06           472 12               511 12               550 GTO 29
356♦LBL 26           395 RCL 05           434 STO IND 05       473 +                512 +                551 1
357 RCL IND 02       396 +                435 ISG 05           474 ENTER↑           513 ENTER↑           552 STO T
358 RCL IND 07       397 1 E3             436♦LBL 07           475 ENTER↑           514 ENTER↑           553 RDN
359 *                398 /                437 ISG 07           476 RCL 05           515 RCL 05           554♦LBL 30
360 ST+ IND 03       399 +                438 GTO 33           477 +                516 +                555 RCL X
361 2                400 STO 07           439 RCL 01           478 1 E3             517 X<>Y             556 ST/ T
362 ST+ 03           401 STO 01           440 FRC              479 /                518 1 E3             557 CLX
363 ST+ 07           402 RCL 04           441 1 E3             480 +                519 /                558 RCL Z
364 RCL 03           403 12               442 *                481 STO 07           520 +                559 ST* T
365 RCL 04           404 +                443 RCL 04           482 0                521 STO 07           560 RDN
366 2                405 STO 05           444 2                483 STO 02           522 RCL 01           561 DSE Y
367 *                406 0                445 *                484♦LBL 35           523 RCL IND 07       562 DSE Y
368 -                407 STO 02           446 -                485 "A"              524 *                563 GTO 30
369 RCL 01           408 STO 03           447 13               486 FIX 0            525 DSE 07           564 RCL Z
370 -                409♦LBL 33           448 -                487 CF 29            526♦LBL 37           565 RTN
371 15               410 1                449 STO 05           488 ARCL 02          527 RCL IND 07       566♦LBL 28
372 X>Y?             411 STO 10           450 RCL 04           489 "⊢= "            528 +                567 1
373 GTO 26           412 0                451 12               490 RCL IND 07       529 RCL 01           568 RTN
374 RCL 01           413 STO 06           452 +                491 XEQ "FMT"        530 *                569 GTO 30
375 RCL 05           414 RCL 07           453 ENTER↑           492 ARCL X           531 DSE 07           570 RTN
376 X=Y?             415 STO 01           454 ENTER↑           493 AVIEW            532 GTO 37           571♦LBL 29
377 GTO 45           416♦LBL 32           455 RCL 05           494 FC? 55           533 RCL IND 07       572 1
378 GTO 05           417 XEQ 31           456 +                495 STOP             534 +                573 RTN
379♦LBL 24           418 RCL IND 01       457 1 E3             496 1                535 XEQ "FMT"        574 .END.
380 FS? 00           419 *                458 /                497 ST+ 02           536 "YBAR= "
381 GTO 25           420 RCL 10           459 +                498 ISG 07           537 ARCL X
```

truncated at this degree, m, and a satisfactory fit has been obtained.

Register usage

The program, plus the FMT subroutine used here, requires 126 registers of memory. To fit an nth-degree polynomial, $18 + 3n$ data registers are also required. This necessitates at least two memory modules, enabling a 15th-degree polynomial to be fitted. With one or two more modules, a 37th- or 58th-degree polynomial may be fitted.

No other accessory is required, although a printer is convenient (the program is printer-compatible). A cardreader or wand is desirable if the program is to be frequently loaded. The program is available from the author in magnetic card form if readers send four blank HP magnetic cards with a request to the author.

Example

Dorn and McCracken [5] give the example of the data of Table II. These values were obtained from:

$$y = x^6 + x^5 + 2x^4 + 3x^3 + 5x^2 + 10x + 40$$

Using the program of Ref. 2, and fitting a sixth-degree polynomial (we could try higher), the following values for the coefficients were obtained:

$$\begin{aligned} a_0 &= 84.7357 \quad (\text{cf. } 40) \\ a_1 &= -63.3921 \quad (\text{cf. } 10) \\ a_2 &= 44.2288 \quad (\text{cf. } 5) \\ a_3 &= -6.4036 \quad (\text{cf. } 3) \\ a_4 &= 3.1161 \quad (\text{cf. } 2) \\ a_5 &= 0.9359 \quad (\text{cf. } 1) \\ a_6 &= 1.0014 \quad (\text{cf. } 1) \end{aligned}$$

These are very different from the values used to gen-

Execution of the program:

Key in	Press	Output
	XEQ 'POLY'	"HOW MANY POINTS?"
$N+1$ (Number of points)	R/S	"MAXIMUM DEGREE?"
$n(\leq N)$	R/S	"INITIAL X?"
x_0	R/S	"FINAL X?"
x_n	R/S	"Y0 ="
y_0	R/S	"Y1 ="
⋮	⋮	⋮
y_N	R/S	"DEGREE?"
$m(\leq n)$	R/S	"A0 ="
	R/S	"A1 ="
	R/S	"A2 ="
	⋮	⋮
	R/S	"Am ="

To obtain y for any given x, use the following procedure. The value obtained is called y bar (or $\bar{y}$), a conditional mean value for that particular x, as projected by the regression polynomial.

In USER mode:

Key in	Press	Output
	C	"X ="
x	R/S	"Y BAR ="

Repeat as required.

To obtain a polynomial of different degree:

In USER mode:

Key in	Press	Output
	B	"DEGREE?"
m	R/S	"A0 ="
	R/S	"A1 ="
	⋮	⋮
	R/S	"Am ="

Repeat as desired.

erate the data. The conditional means for the first four entries in Table II are:

y bar (1) = 64.2227 (cf. 62)
(2) = 227.5357 (cf. 232)
(3) = 1,329.5882 (cf. 1,330)
(4) = 5,986.9122 (cf. 5,984)

Clearly, even with a degree of as little as six, there has been a severe loss of accuracy.

When the problem was repeated, using the program of this article, the results obtained were:

$a_0 =$ 40.0155 (cf. 40)
$a_1 =$ 9.9774 (cf. 10)
$a_2 =$ 5.0125 (cf. 5)
$a_3 =$ 2.9968 (cf. 3)
$a_4 =$ 2.0004 (cf. 2)
$a_5 =$ 1.0000 (cf. 1)
$a_6 =$ 1.0000 (cf. 1)

and y bar (1) = 62.0026 (cf. 62)
(2) = 232.0007 (cf. 232)
(3) = 1,330.0017 (cf. 1,330)
(4) = 5,984.0022 (cf. 5,984)

These are obviously very much closer to the values that generated the data. It is also worth noting that the runtime of the program of this article with this example was 7 min; that of the program of Ref. 2 was 20 min.

The conclusion is that, wherever possible, when a polynomial least-squares treatment of data is to be used, the data should be obtained from equal spacing of the independent variable, and fitting should be done with orthogonal polynomials. Otherwise, if high-degree polynomials are used, the error of calculation may be greater than the error of measurement, and this should never be so.

Values for the two variables in the polynomial example of Dorn and McCracken Table II

x	y	x	y
1	62	8	305,080
2	232	9	606,334
3	1,330	10	1,123,640
4	5,984	11	1,966,642
5	20,590	12	3,282,352
6	57,952	13	5,262,830
7	140,642	14	8,153,584

For TI users

The TI program is not a direct translation of the HP program, inasmuch as the TI does not have the storage capacity used by the HP 41C program. However, the TI program carries out similar calculations.

The TI program is limited to 29 y values, and while it will determine the goodness of fit of any degree orthogonal polynomial up to 10, the program will calculate the regression coefficients for a maximum of a fifth-degree equation.

Data are entered and the program calculates the goodness of fit of successive-degree polynomials. When a satisfactory fit is obtained, the program calculates the regression coefficients, the a_n values, for the degree polynomial selected by the engineer:

$$y = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$$

For instance, the following values are the results of the equation:

$$y = 40 + x + x^2 + x^3 + x^4$$

x	1	2	3	4	5	6	7	8
y	44	70	160	380	820	1594	2840	4720

If these data are entered, the program gives the following (rounded off to 5 decimal places):

Degree	Variation removed	Total variation removed	Correlation coefficient
1	0.79937	0.79937	0.89408
2	0.18960	0.98898	0.99447
3	0.01093	0.99991	0.99995
4	0.00009	1.00000	1.00000

Calculation of regression coefficients for a fourth degree equation: (inputted as 4 key *C*) gives:

a_o	40.00000081
a_1	0.99999878
a_2	1.00000001
a_3	0.99999991
a_4	1.00000000

Listing for TI version—program 1 **Table III**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	053	55	÷	106	33	X²	159	42	STO	212	09	9
001	11	A	054	43	RCL	107	43	RCL	160	00	00	213	22	INV
002	32	X⇌T	055	00	00	108	00	00	161	76	LBL	214	44	SUM
003	47	CMS	056	95	=	109	85	+	162	32	X⇌T	215	00	00
004	01	1	057	42	STO	110	01	1	163	43	RCL	216	43	RCL
005	42	STO	058	58	58	111	95	=	164	57	57	217	00	00
006	00	00	059	76	LBL	112	65	×	165	75	-	218	32	X⇌T
007	32	X⇌T	060	14	D	113	43	RCL	166	43	RCL	219	43	RCL
008	72	ST*	061	01	1	114	55	55	167	00	00	220	57	57
009	00	00	062	44	SUM	115	55	÷	168	85	+	221	77	GE
010	44	SUM	063	57	57	116	53	(	169	01	1	222	32	X⇌T
011	59	59	064	42	STO	117	43	RCL	170	95	=	223	02	2
012	33	X²	065	00	00	118	56	56	171	65	×	224	65	×
013	44	SUM	066	00	0	119	85	+	172	53	(	225	43	RCL
014	58	58	067	42	STO	120	43	RCL	173	43	RCL	226	57	57
015	91	R/S	068	59	59	121	00	00	174	57	57	227	85	+
016	76	LBL	069	76	LBL	122	54	)	175	85	+	228	01	1
017	22	INV	070	23	LNX	123	95	=	176	43	RCL	229	95	=
018	32	X⇌T	071	73	RC*	124	42	STO	177	00	00	230	42	STO
019	01	1	072	00	00	125	55	55	178	54	)	231	52	52
020	44	SUM	073	32	X⇌T	126	01	1	179	55	÷	232	01	1
021	00	00	074	01	1	127	44	SUM	180	43	RCL	233	42	STO
022	32	X⇌T	075	44	SUM	128	00	00	181	00	00	234	00	00
023	72	ST*	076	00	00	129	43	RCL	182	55	÷	235	76	LBL
024	00	00	077	32	X⇌T	130	00	00	183	53	(	236	34	√X
025	44	SUM	078	74	SM*	131	32	X⇌T	184	43	RCL	237	43	RCL
026	59	59	079	00	00	132	43	RCL	185	00	00	238	57	57
027	33	X²	080	44	SUM	133	57	57	186	85	+	239	85	+
028	44	SUM	081	59	59	134	77	GE	187	01	1	240	43	RCL
029	58	58	082	43	RCL	135	33	X²	188	54	)	241	00	00
030	91	R/S	083	00	00	136	03	3	189	65	×	242	95	=
031	61	GTO	084	32	X⇌T	137	00	0	190	43	RCL	243	65	×
032	22	INV	085	43	RCL	138	85	+	191	53	53	244	43	RCL
033	76	LBL	086	56	56	139	43	RCL	192	94	+/-	245	52	52
034	12	B	087	67	EQ	140	57	57	193	95	=	246	55	÷
035	43	RCL	088	42	STO	141	95	=	194	42	STO	247	43	RCL
036	59	59	089	61	GTO	142	42	STO	195	53	53	248	00	00
037	55	÷	090	23	LNX	143	00	00	196	32	X⇌T	249	55	÷
038	43	RCL	091	76	LBL	144	43	RCL	197	03	3	250	53	(
039	00	00	092	42	STO	145	55	55	198	00	0	251	43	RCL
040	42	STO	093	73	RC*	146	65	×	199	44	SUM	252	56	56
041	56	56	094	00	00	147	43	RCL	200	00	00	253	75	-
042	95	=	095	44	SUM	148	59	59	201	73	RC*	254	43	RCL
043	42	STO	096	59	59	149	95	=	202	00	00	255	00	00
044	30	30	097	43	RCL	150	72	ST*	203	65	×	256	54	)
045	42	STO	098	56	56	151	00	00	204	32	X⇌T	257	95	=
046	40	40	099	35	1/X	152	43	RCL	205	85	+	258	42	STO
047	43	RCL	100	42	STO	153	30	30	206	43	RCL	259	52	52
048	58	58	101	55	55	154	42	STO	207	54	54	260	01	1
049	75	-	102	01	1	155	54	54	208	95	=	261	44	SUM
050	43	RCL	103	42	STO	156	01	1	209	42	STO	262	00	00
051	59	59	104	00	00	157	42	STO	210	54	54	263	43	RCL
052	33	X²	105	76	LBL	158	53	53	211	02	2	264	00	00

(Continued) Table III

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
265	32	X:T	308	43	RCL	351	44	SUM	394	42	STO	437	43	RCL
266	43	RCL	309	56	56	352	51	51	395	50	50	438	42	42
267	57	57	310	33	X²	353	43	RCL	396	43	RCL	439	65	×
268	77	GE	311	75	-	354	53	53	397	40	40	440	53	(
269	34	√X	312	43	RCL	355	55	÷	398	75	-	441	43	RCL
270	03	3	313	00	00	356	43	RCL	399	43	RCL	442	50	50
271	09	9	314	33	X²	357	58	58	400	41	41	443	33	X²
272	44	SUM	315	54	)	358	95	=	401	65	×	444	75	-
273	00	00	316	95	=	359	99	PRT	402	43	RCL	445	53	(
274	43	RCL	317	42	STO	360	43	RCL	403	50	50	446	43	RCL
275	52	52	318	53	53	361	51	51	404	95	=	447	56	56
276	65	×	319	01	1	362	55	÷	405	42	STO	448	33	X²
277	43	RCL	320	44	SUM	363	43	RCL	406	40	40	449	75	-
278	54	54	321	00	00	364	58	58	407	01	1	450	01	1
279	95	=	322	43	RCL	365	95	=	408	22	INV	451	54	)
280	72	ST*	323	00	00	366	99	PRT	409	67	EQ	452	55	÷
281	00	00	324	32	X:T	367	34	√X	410	43	RCL	453	01	1
282	43	RCL	325	43	RCL	368	99	PRT	411	43	RCL	454	02	2
283	56	56	326	57	57	369	98	ADV	412	40	40	455	54	)
284	42	STO	327	77	GE	370	91	R/S	413	99	PRT	456	95	=
285	53	53	328	35	1/X	371	14	D	414	43	RCL	457	42	STO
286	01	1	329	03	3	372	76	LBL	415	41	41	458	40	40
287	42	STO	330	09	9	373	13	C	416	99	PRT	459	02	2
288	00	00	331	44	SUM	374	42	STO	417	98	ADV	460	22	INV
289	76	LBL	332	00	00	375	00	00	418	91	R/S	461	67	EQ
290	35	1/X	333	43	RCL	376	32	X:T	419	76	LBL	462	44	SUM
291	43	RCL	334	53	53	377	05	5	420	43	RCL	463	43	RCL
292	53	53	335	65	×	378	22	INV	421	43	RCL	464	40	40
293	65	×	336	73	RC*	379	77	GE	422	41	41	465	99	PRT
294	43	RCL	337	00	00	380	15	E	423	75	-	466	43	RCL
295	00	00	338	33	X²	381	43	RCL	424	43	RCL	467	41	41
296	33	X²	339	55	÷	382	57	57	425	42	42	468	99	PRT
297	55	÷	340	53	(	383	22	INV	426	65	×	469	43	RCL
298	53	(	341	02	2	384	77	GE	427	02	2	470	42	42
299	43	RCL	342	65	×	385	15	E	428	65	×	471	99	PRT
300	57	57	343	43	RCL	386	43	RCL	429	43	RCL	472	98	ADV
301	85	+	344	57	57	387	56	56	430	50	50	473	76	LBL
302	43	RCL	345	85	+	388	85	+	431	95	=	474	44	SUM
303	00	00	346	01	1	389	01	1	432	42	STO	475	91	R/S
304	54	)	347	54	)	390	95	=	433	41	41			
305	33	X²	348	95	=	391	55	÷	434	43	RCL			
306	65	×	349	42	STO	392	02	2	435	40	40			
307	53	(	350	53	53	393	95	=	436	85	+			

Listing for TI version—program 2 **Table IV**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	015	51	51	030	41	41	045	95	=	060	43	RCL
001	13	C	016	43	RCL	031	85	+	046	42	STO	061	50	50
002	43	RCL	017	42	42	032	43	RCL	047	41	41	062	65	×
003	56	56	018	75	-	033	43	43	048	43	RCL	063	43	RCL
004	33	X²	019	43	RCL	034	65	×	049	40	40	064	51	51
005	65	×	020	43	43	035	53	(	050	75	-	065	54	)
006	03	3	021	65	×	036	03	3	051	43	RCL	066	95	=
007	75	-	022	03	3	037	65	×	052	43	43	067	42	STO
008	07	7	023	65	×	038	43	RCL	053	65	×	068	40	40
009	95	=	024	43	RCL	039	50	50	054	53	(	069	03	3
010	55	÷	025	50	50	040	33	X²	055	43	RCL	070	22	INV
011	02	2	026	95	=	041	75	-	056	50	50	071	67	EQ
012	00	0	027	42	STO	042	43	RCL	057	45	Yˣ	072	22	INV
013	95	=	028	42	42	043	51	51	058	03	3	073	43	RCL
014	42	STO	029	43	RCL	044	54	)	059	75	-	074	40	40

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
075	99	PRT	141	65	×	208	23	LNX	274	45	45	341	04	4
076	43	RCL	142	53	(	209	43	RCL	275	65	×	342	75	-
077	41	41	143	04	4	210	40	40	276	05	5	343	03	3
078	99	PRT	144	65	×	211	99	PRT	277	65	×	344	65	×
079	43	RCL	145	43	RCL	212	43	RCL	278	43	RCL	345	43	RCL
080	42	42	146	50	50	213	41	41	279	50	50	346	50	50
081	99	PRT	147	45	Y^x	214	99	PRT	280	95	=	347	33	X^2
082	43	RCL	148	03	3	215	43	RCL	281	42	STO	348	65	×
083	43	43	149	75	-	216	42	42	282	44	44	349	43	RCL
084	99	PRT	150	02	2	217	99	PRT	283	43	RCL	350	51	51
085	98	ADV	151	65	×	218	43	RCL	284	43	43	351	85	+
086	91	R/S	152	43	RCL	219	43	43	285	85	+	352	43	RCL
087	76	LBL	153	50	50	220	99	PRT	286	43	RCL	353	52	52
088	22	INV	154	65	×	221	43	RCL	287	45	45	354	54	)
089	43	RCL	155	43	RCL	222	44	44	288	65	×	355	95	=
090	56	56	156	51	51	223	99	PRT	289	53	(	356	42	STO
091	33	X^2	157	54	)	224	98	ADV	290	01	1	357	41	41
092	65	×	158	95	=	225	91	R/S	291	00	0	358	43	RCL
093	03	3	159	42	STO	226	76	LBL	292	65	×	359	40	40
094	75	-	160	41	41	227	23	LNX	293	43	RCL	360	75	-
095	01	1	161	43	RCL	228	43	RCL	294	50	50	361	43	RCL
096	03	3	162	40	40	229	56	56	295	33	X^2	362	45	45
097	95	=	163	85	+	230	33	X^2	296	75	-	363	65	×
098	55	÷	164	43	RCL	231	75	-	297	43	RCL	364	53	(
099	01	1	165	44	44	232	07	7	298	51	51	365	43	RCL
100	04	4	166	65	×	233	95	=	299	54	)	366	50	50
101	95	=	167	53	(	234	65	×	300	95	=	367	45	Y^x
102	42	STO	168	43	RCL	235	05	5	301	42	STO	368	05	5
103	51	51	169	50	50	236	55	÷	302	43	43	369	75	-
104	43	RCL	170	45	Y^x	237	01	1	303	43	RCL	370	43	RCL
105	43	43	171	04	4	238	08	8	304	42	42	371	50	50
106	75	-	172	75	-	239	95	=	305	75	-	372	45	Y^x
107	43	RCL	173	43	RCL	240	42	STO	306	43	RCL	373	03	3
108	44	44	174	50	50	241	51	51	307	45	45	374	65	×
109	65	×	175	33	X^2	242	01	1	308	65	×	375	43	RCL
110	04	4	176	65	×	243	05	5	309	53	(	376	51	51
111	65	×	177	43	RCL	244	65	×	310	01	1	377	85	+
112	43	RCL	178	51	51	245	43	RCL	311	00	0	378	43	RCL
113	50	50	179	85	+	246	56	56	312	65	×	379	50	50
114	95	=	180	03	3	247	45	Y^x	313	43	RCL	380	65	×
115	42	STO	181	65	×	248	04	4	314	50	50	381	43	RCL
116	43	43	182	53	(	249	75	-	315	45	Y^x	382	52	52
117	43	RCL	183	43	RCL	250	02	2	316	03	3	383	54	)
118	42	42	184	56	56	251	03	3	317	75	-	384	95	=
119	85	+	185	45	Y^x	252	00	0	318	03	3	385	42	STO
120	43	RCL	186	04	4	253	65	×	319	65	×	386	40	40
121	44	44	187	75	-	254	43	RCL	320	43	RCL	387	43	RCL
122	65	×	188	01	1	255	56	56	321	50	50	388	40	40
123	53	(	189	00	0	256	33	X^2	322	65	×	389	99	PRT
124	06	6	190	65	×	257	85	+	323	43	RCL	390	43	RCL
125	65	×	191	43	RCL	258	04	4	324	51	51	391	41	41
126	43	RCL	192	56	56	259	00	0	325	54	)	392	99	PRT
127	50	50	193	33	X^2	260	07	7	326	95	=	393	43	RCL
128	33	X^2	194	85	+	261	95	=	327	42	STO	394	42	42
129	75	-	195	09	9	262	55	÷	328	42	42	395	99	PRT
130	43	RCL	196	54	)	263	01	1	329	43	RCL	396	43	RCL
131	51	51	197	55	÷	264	00	0	330	41	41	397	43	43
132	54	)	198	05	5	265	00	0	331	85	+	398	99	PRT
133	95	=	199	06	6	266	08	8	332	43	RCL	399	43	RCL
134	42	STO	200	00	0	267	95	=	333	45	45	400	44	44
135	42	42	201	54	)	268	42	STO	334	65	×	401	99	PRT
136	43	RCL	202	95	=	269	52	52	335	53	(	402	43	RCL
137	41	41	203	42	STO	270	43	RCL	336	05	5	403	45	45
138	75	-	204	40	40	271	44	44	337	65	×	404	99	PRT
139	43	RCL	205	04	4	272	75	-	338	43	RCL	405	98	ADV
140	44	44	206	22	INV	273	43	RCL	339	50	50	406	91	R/S
			207	67	EQ				340	45	Y^x			

User instructions for the TI version **Table V**

Step	Input	Key	Output
2. Input data	x_i	**x⇌t**	
	y_i	**A** (for first *y* value only)	
		R/S (for subsequent *y* values)	
3. When all data are entered		**B**	Starts calculation
4. Calculate output			a. Fraction of the sum of squares of deviation accounted for by that degree b. Total fraction of the sum of squares of deviation accounted for by the equation to that degree c. Correlation coefficient for thee equation to that degree
5. Continue output calculations for next degree		**R/S**	Same as step 1
6. Calculate regression coefficients n*		**C**	a_0, a_1, a_2, etc. (to a_n)
7. Load program 2†		**C**	Same as step 6

*When a satisfactory fitness is obtained (based upon the highest value of correlation coefficient, calculated previously), the user enters *n*, the degree of the equation to be calculated. This value cannot be higher than 5, or higher than the maximum goodness of fit calculated. If the number entered is higher than 5, or greater than the maximum goodness of fit, the calculator will show a flashing display. The flashing may be cleared by pressing the **CLR** key. Then enter the correct value of *n*, followed by pressing the **C** key.

†If a first- or second-degree equation is to be calculated, the results will be obtained directly (i.e., with only the first program loaded). If a higher degree is to be used, the calculator will display the number "2," indicating that the second program should be entered. Pressing the **C** key will complete the calculation.

Acknowledgment

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Section III
Physical Properties Correlation

Program predicts critical properties of organic compounds
Predict thermal conductivities of gas mixtures and liquids
Predict thermal conductivities of liquid mixtures
Predict equation-of-state variables
Predict gas-phase diffusion coefficients
Predict liquid-phase diffusion coefficients

Program predicts critical properties of organic compounds

Written for the TI-59, this method determines critical temperature, pressure, volume and compressibility, using the Lydersen method.

Jacob Zabicky, Ben-Gurion University of the Negev

☐ The deserved popularity of the Lydersen method [*1–3*] for estimating critical properties of organic compounds is based on its simplicity and overall reliability. The only data required are the normal boiling point, T_b, the molecular weight, M, and the structural formula of the compound.

Lydersen's equations

When the chosen units are Kelvin for temperature, atmospheres for pressure and dm^3/mole for molar volume, the following formulas are used:

$$T_c = T_b/(0.567 + \Sigma\Delta_T - (\Sigma\Delta_T)^2) \quad (1)$$
$$p_c = M/(0.34 + \Sigma\Delta_p)^2 \quad (2)$$
$$v_c = 0.04 + \Sigma\Delta_v/1{,}000 \quad (3)$$

where T_c is critical temperature, p_c is critical pressure and v_c is critical volume. The subscripts T, p and v are used to refer to critical temperature, pressure and volume, respectively.

The critical compressibility factor, z_c, is then estimated by:

$$z_c = \frac{p_c v_c}{RT_c} \quad (4)$$

where R is the ideal gas constant.

Atomic and functional groups used in determining critical properties **Table I**

Group	Code	Printout[a]	Group	Code	Printout[a]
$-CH_3$	0. 08	CH3	-O- open-chain ether	0. 25	-O-Q
$-CH_2-$ open-chain	0. 08	CH2Q	-O- ring ether	0. 26	-O-R
$-CH_2-$ ring	0. 09	CH2R	)C=O open-chain ketone	0. 27	KETQ
)CH- open-chain	0. 1	CH Q	)C=O ring ketone	0. 28	KETR
)CH- ring	0. 11	CH R	-CHO aldehyde	0. 29	CH=O
)CH- angular	0. 12[b]	CHR2	-COOH	0. 3	COOH
)C(open-chain	0. 13	)C(Q	-COOR ester	0. 31	COOE
)C(ring	0. 14	)C(R	=O other types	0. 32	=O V
$=CH_2$	0. 15	=CH2	$-NH_2$	0. 33	-NH2
=CH- open-chain	0. 15	=CHQ	-NH- open-chain	0. 34	)NHQ
=C(open-chain	0. 16	=C(Q	-NH- ring	0. 35	)NHR
=C= open-chain	0. 16	=C=Q	)N- open-chain	0. 36	)N-Q
=C ring, all types	0. 17	=C R	)N- ring	0. 37	)N-R
≡CH	0. 18	ΣCH	-C≡N	0. 38	-CN
≡C- open-chain	0. 18	ΣC-Q	$-NO_2$	0. 39	-NO2
≡C- ring	0. 18	ΣC-R	-SH	0. 4	-SH
-F	0. 19	-F	-S- open-chain	0. 4	-S-Q
-Cl	0. 2	-CL	-S- ring	0. 41	-S-R
-Br	0. 21	-BR	=S	0. 42	=S
-I	0. 22	-I	)Si(	c	
-OH alcohol	0. 23	-OHA	)B-	d	
-OH phenol	0. 24	-OHP			

[a]Q=open-chain, R=ring, Σ=triple bond, A=alcohol, P=phenol, V=various types of double-bonded oxygen not listed above.
[b]Proposed by Fishtine [*4*] when the CH group is shared by two saturated rings.
[c]Not included in the program; Δ_T=0.03, Δ_p=0.54.
[d]Not included in the program; Δ_T=0.03.

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TI-59 program estimates critical properties of many organic compounds

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
000	76	LBL	063	00	0	126	15	E	189	01	1	252	01	1	315	07	7
001	19	D'	064	00	0	127	98	ADV	190	05	5	253	00	0	316	09	9
002	44	SUM	065	49	PRD	128	98	ADV	191	05	5	254	00	0	317	01	1
003	03	03	066	02	02	129	25	CLR	192	05	5	255	00	0	318	19	D'
004	61	GTO	067	65	×	130	42	STO	193	03	3	256	00	0	319	06	6
005	00	00	068	43	RCL	131	03	03	194	04	4	257	17	B'	320	94	+/-
006	11	11	069	01	01	132	42	STO	195	17	B'	258	05	5	321	19	D'
007	76	LBL	070	95	=	133	04	04	196	01	1	259	07	7	322	06	6
008	17	B'	071	44	SUM	134	42	STO	197	19	D'	260	03	3	323	04	4
009	42	STO	072	03	03	135	05	05	198	07	7	261	00	0	324	03	3
010	03	03	073	43	RCL	136	91	R/S	199	09	9	262	00	0	325	02	2
011	69	OP	074	02	02	137	76	LBL	200	09	9	263	94	+/-	326	00	0
012	21	21	075	59	INT	138	16	A'	201	06	6	264	19	D'	327	00	0
013	43	RCL	076	22	INV	139	94	+/-	202	07	7	265	09	9	328	04	4
014	01	01	077	44	SUM	140	99	PRT	203	06	6	266	02	2	329	02	2
015	65	×	078	02	02	141	94	+/-	204	08	8	267	00	0	330	17	B'
016	93	.	079	55	÷	142	71	SBR	205	19	D'	268	00	0	331	02	2
017	00	0	080	01	1	143	00	00	206	69	OP	269	94	+/-	332	00	0
018	01	1	081	00	0	144	34	34	207	31	31	270	19	D'	333	03	3
019	95	=	082	00	0	145	02	2	208	03	3	271	09	9	334	01	1
020	32	X:T	083	00	0	146	94	+/-	209	01	1	272	06	6	335	02	2
021	43	RCL	084	65	×	147	49	PRD	210	19	D'	273	05	5	336	03	3
022	03	03	085	43	RCL	148	01	01	211	03	3	274	00	0	337	00	0
023	76	LBL	086	01	01	149	61	GTO	212	02	2	275	00	0	338	03	3
024	18	C'	087	95	=	150	00	00	213	00	0	276	19	D'	339	17	B'
025	69	OP	088	44	SUM	151	47	47	214	00	0	277	08	8	340	05	5
026	04	04	089	04	04	152	76	LBL	215	19	D'	278	02	2	341	06	6
027	32	X:T	090	43	RCL	153	10	E'	216	69	OP	279	03	3	342	03	3
028	69	OP	091	02	02	154	25	CLR	217	31	31	280	01	1	343	01	1
029	06	06	092	50	I×I	155	07	7	218	00	0	281	03	3	344	02	2
030	92	RTN	093	65	×	156	42	STO	219	09	9	282	19	D'	345	03	3
031	76	LBL	094	43	RCL	157	01	01	220	00	0	283	02	2	346	03	3
032	11	A	095	01	01	158	01	1	221	00	0	284	00	0	347	04	4
033	99	PRT	096	95	=	159	05	5	222	19	D'	285	19	D'	348	17	B'
034	42	STO	097	44	SUM	160	02	2	223	06	6	286	02	2	349	01	1
035	00	00	098	05	05	161	03	3	224	03	3	287	09	9	350	19	D'
036	59	INT	099	92	RTN	162	00	0	225	09	9	288	09	9	351	03	3
037	22	INV	100	48	EXC	163	04	4	226	09	9	289	94	+/-	352	00	0
038	44	SUM	101	00	00	164	00	0	227	94	+/-	290	19	D'	353	01	1
039	00	00	102	32	X:T	165	00	0	228	19	D'	291	01	1	354	94	+/-
040	42	STO	103	01	1	166	17	B'	229	07	7	292	19	D'	355	19	D'
041	01	01	104	04	4	167	69	OP	230	07	7	293	02	2	356	01	1
042	01	1	105	67	EQ	168	31	31	231	01	1	294	06	6	357	19	D'
043	00	0	106	01	01	169	06	6	232	05	5	295	01	1	358	02	2
044	00	0	107	18	18	170	06	6	233	02	2	296	07	7	359	00	0
045	49	PRD	108	01	1	171	94	+/-	234	03	3	297	03	3	360	01	1
046	00	00	109	94	+/-	172	19	D'	235	00	0	298	07	7	361	05	5
047	73	RC*	110	49	PRD	173	01	1	236	00	0	299	03	3	362	03	3
048	00	00	111	00	00	174	19	D'	237	17	B'	300	04	4	363	01	1
049	42	STO	112	32	X:T	175	03	3	238	69	OP	301	17	B'	364	00	0
050	02	02	113	48	EXC	176	00	0	239	31	31	302	01	1	365	00	0
051	59	INT	114	00	00	177	01	1	240	02	2	303	19	D'	366	17	B'
052	22	INV	115	61	GTO	178	94	+/-	241	06	6	304	01	1	367	01	1
053	44	SUM	116	00	00	179	19	D'	242	06	6	305	05	5	368	06	6
054	02	02	117	60	60	180	01	1	243	94	+/-	306	02	2	369	00	0
055	29	CP	118	01	1	181	19	D'	244	19	D'	307	03	3	370	01	1
056	22	INV	119	94	+/-	182	03	3	245	69	OP	308	06	6	371	00	0
057	77	GE	120	49	PRD	183	05	5	246	31	31	309	04	4	372	03	3
058	01	01	121	02	02	184	03	3	247	01	1	310	03	3	373	19	D'
059	00	00	122	61	GTO	185	05	5	248	19	D'	311	02	2	374	04	4
060	55	÷	123	01	01	186	19	D'	249	02	2	312	17	B'	375	09	9
061	01	1	124	12	12	187	05	5	250	00	0	313	08	8	376	00	0
062	00	0	125	76	LBL	188	06	6	251	02	2	314	06	6	377	09	9

with high accuracy and uses partitioning 5 Op 17 **Table II**

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
378	07	7	405	73	RC*	432	18	C'	459	53	(	486	53	(	513	05	05
379	19	D'	406	01	01	433	91	R/S	460	43	RCL	487	93	.	514	55	÷
380	69	OP	407	69	OP	434	76	LBL	461	03	03	488	03	3	515	01	1
381	31	31	408	03	03	435	13	C	462	75	-	489	04	4	516	00	0
382	02	2	409	69	OP	436	42	STO	463	33	X²	490	85	+	517	54	)
383	06	6	410	21	21	437	06	06	464	85	+	491	43	RCL	518	32	X:T
384	06	6	411	73	RC*	438	32	X:T	465	93	.	492	04	04	519	04	4
385	94	+/-	412	01	01	439	25	CLR	466	05	5	493	54	)	520	02	2
386	19	D'	413	69	OP	440	03	3	467	06	6	494	33	X²	521	01	1
387	01	1	414	04	04	441	00	0	468	07	7	495	54	)	522	05	5
388	19	D'	415	69	OP	442	04	4	469	54	)	496	32	X:T	523	02	2
389	06	6	416	05	05	443	03	3	470	54	)	497	03	3	524	00	0
390	04	4	417	97	DSZ	444	18	C'	471	32	X:T	498	03	3	525	02	2
391	03	3	418	00	00	445	91	R/S	472	03	3	499	01	1	526	07	7
392	06	6	419	04	04	446	76	LBL	473	07	7	500	05	5	527	18	C'
393	00	0	420	03	03	447	14	D	474	01	1	501	02	2	528	95	=
394	00	0	421	91	R/S	448	25	CLR	475	05	5	502	00	0	529	32	X:T
395	00	0	422	76	LBL	449	01	1	476	02	2	503	01	1	530	04	4
396	00	0	423	12	B	450	02	2	477	00	0	504	03	3	531	06	6
397	17	B'	424	42	STO	451	93	.	478	02	2	505	18	C'	532	01	1
398	03	3	425	07	07	452	01	1	479	06	6	506	65	×	533	05	5
399	42	STO	426	32	X:T	453	09	9	480	18	C'	507	53	(	534	00	0
400	00	00	427	25	CLR	454	55	÷	481	65	×	508	93	.	535	00	0
401	69	OP	428	03	3	455	53	(	482	53	(	509	00	0	536	00	0
402	00	00	429	07	7	456	43	RCL	483	43	RCL	510	04	4	537	00	0
403	69	OP	430	01	1	457	07	07	484	06	06	511	85	+	538	18	C'
404	21	21	431	04	4	458	55	÷	485	55	÷	512	43	RCL	539	91	R/S

Note: For operation without printer, write $x \rightleftharpoons t$ (code 32) in locations 479, 504, 526, 537, and **R/S** (code 91) in 480, 505, 527, 538. Pressing **D, R/S, R/S, R/S** will yield the values of T_c, p_c, v_c and z_c in succession.

Data registers used in running the program. Registers 08 to 48 must be punched in **Table III**

Number	Content	Number	Content	Number	Content
00	Used	17	11.15436	34	31.13537
01	Used	18	5.15336	35	24.09027
02	Used	19	18.22418	36	14.17042
03	$\Sigma\ \Delta_T$	20	17.32049	37	7.13032
04	$\Sigma\ \Delta_p$	21	10.5007	38	60.3608
05	$\Sigma\ \Delta_v$	22	12.83095	39	55.42078
06	M	23	82.06018	40	15.27055
07	T_b	24	-31.02003	41	8.24045
08	20.22755	25	21.1602	42	3.24047
09	13.184445	26	14.12008	43	3464323317
10	12.21051	27	40.2906	44	3100152340
11	12.19246	28	33.2005	45	3564352431
12	64.19246	29	48.33073	46	2200000000
13	0.21041	30	85.4008	47	7764373524
14	-7.15431	31	47.4708	48	3327170014
15	18.19845	32	20.12011		
16	0.19836	33	31.09528		

Note: Use partition 5 **Op** 17

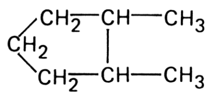
Lydersen's method determines the critical properties by adding up atomic and structural-group contributions. Such additions are carried out over all structural groups in a compound. The Δ values in Eq. 1–3 represent those contributions. The values are taken from the references listed here, and will not be repeated in this article. The groups used in the program appear in Table I.

The summations are carried out over all the structural groups in the formula of the compound.

For the purposes of the program, the functional groups receive a numerical code, as shown in the table.

User's instructions and two examples; the results are compared with experimental data **Table IV**

Example: Estimate critical properties of *cis*- and *trans*- 1,2-dimethylcyclopentane



(both compounds)

Group	Code	n	$n.x$[a]	Group	n	Code	$n.x$[a]
CH_3—	2	.08	2.08	>CH— ring	2	.11	2.11
—CH_2— ring	3	.09	3.09				

Step	Description	Enter	Press	Display	Printout	
1.	Need a code listing?		E′		Listing of codes	
2.[b]	Initiate *cis* estimate		E	0.	Paper advances	
3.	Enter T_b of *cis* (K)	372.2	B	372.2	372.2	TB
4.	Enter *M* of *cis*	98.189	C	98.189	98.189	MW
5.	Enter groups of *cis*	2.09	A		2.09	
		3.09	A		3.09	
		2.11	A		2.11	
6.	(a) A wrong entry (2.09) was made in Step 5	2.09	A′		-2.09	
	(b) Enter correct value	2.08	A		2.08	
7.[c]	Estimate critical properties		D		564.4602368	TC-K
					32.80731064	PC-A
					0.3755	VC-L
					.2660424411	ZC
2′.	Initiate *trans* estimate (unnecessary)[d]					
3′.	Enter T_b of *trans*	365.	B	365.	365.	TB
4′.	Enter *M* of *trans* (unnecessary)[d]					
5′.-6′.	Enter groups of *trans* (unnecessary)[d]					
7′.[c]	Estimate critical properties		D		553.5410705	TC-K
					32.80731064	PC-A
					0.3755	VC-L
					.2712904016	ZC

Notes: [a]Groups with the same *X* code may be combined by adding their *n* values.
[b]Does not affect stored T_b or *M* values.
[c]Does not affect stored values. Literature values [3] for *cis* and *trans* are, respectively:
T_c = 564.8, 553.2 K; p_c = 34.0, 34.0 atm; v_c = 0.368, 0.362 dm^3/mole; z_c = 0.27, 0.27.
[d]The functional groups and molecular weights of both compounds are the same.
If key **E** is pressed in Step 2′, then the *n.x* values have to be entered in Step 5′.

The three Δ values of a group with code *X* are stored in a condensed form in register 100*X*. For example, the contents of register 38, corresponding to the CN group (code .38) are:

$$R_{38} = 1{,}000\,|\Delta_T| + |\Delta_p| + \frac{\Delta_v}{100{,}000}$$

When the value of a Δ is negative the register content is negative, too.

Accuracy

Hougen et al. [2] reported on the accuracy of the Lydersen method. For estimating T_c, the average deviation from experimental data is 1.0%, based upon 233 compounds. For p_c, the deviation is 3.3% (159 compounds); for v_c, the deviation is 2.4% (141 compounds). For z_c, estimated by Eq. (4), the deviation is 3.4% (121 compounds).

Using the program

The program, written for the TI-59, appears in Table II. Note that 5 **Op** 17 partitioning is used. After loading the program, data registers 08-48 must be punched in (see Table III).

In order to solve a problem, draw the structural formula of the compound, with as much detail as is required by Table I. Write down a list of numbers of the form *n.X* (where *n* is the number of times the group of code *X* appears in the formula) and proceed as illustrated by the two examples shown in Table IV.

A condensed printout of Table I can be obtained by pressing key **E′**. This printout contains listings for the code, and symbols for each group.

For HP-67/97 users

The HP version closely follows the TI program. Table V contains the listing of the HP program, and Table VI offers the user instructions. Use Table I to determine the codes for the different structural groups.

Program listing for HP version **Table V**

Step	Key	Code	Step	Key	Code
001	*LBLa	21 16 11	015	*LBL3	21 03
002	SF0	16 21 00	016	STOI	35 46
003	*LBLA	21 11	017	INT	16 34
004	F1?	16 23 01	018	STOE	35 15
005	GTO3	22 03	019	RCLI	36 46
006	3	03	020	FRC	16 44
007	STOD	35 14	021	1	01
008	R↓	-31	022	0	00
009	SF1	16 21 01	023	0	00
010	0	00	024	×	-35
011	STOA	35 11	025	RCLD	36 14
012	STOB	35 12	026	-	-45
013	STOC	35 13	027	STOI	35 46
014	R↓	-31	028	RCLi	36 45

(Continued) Table V

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
029	INT	16 34	057	RCLE	36 15	085	GTO1	22 01	113	1/X	52	141	8	08
030	1	01	058	×	-35	086	+	-55	114	STOD	35 14	142	2	02
031	EEX	-23	059	RCLB	36 12	087	GTO2	22 02	115	R↓	-31	143	0	00
032	3	03	060	X⇄Y	-41	088	*LBL1	21 01	116	RCLB	36 12	144	7	07
033	÷	-24	061	F0?	16 23 00	089	-	-45	117	.	-62	145	÷	-24
034	RCLE	36 15	062	GTO1	22 01	090	*LBL2	21 02	118	3	03	146	PRTX	-14
035	×	-35	063	+	-55	091	STOC	35 13	119	4	04	147	SPC	16-11
036	RCLA	36 11	064	GTO2	22 02	092	CF0	16 22 00	120	+	-55	148	CF1	16 22 01
037	X⇄Y	-41	065	*LBL1	21 01	093	R/S	51	121	X²	53	149	R/S	51
038	F0?	16 23 00	066	-	-45	094	*LBLB	21 12	122	÷	-24	150	*LBLD	21 14
039	GTO1	22 01	067	*LBL2	21 02	095	2	02	123	PRTX	-14	151	RCLA	36 11
040	+	-55	068	STOB	35 12	096	7	07	124	RCLD	36 14	152	RCLB	36 12
041	GTO2	22 02	069	RCLi	36 45	097	3	03	125	×	-35	153	RCLC	36 13
042	*LBL1	21 01	070	FRC	16 44	098	.	-62	126	STOD	35 14	154	R/S	51
043	-	-45	071	1	01	099	1	01	127	RCLC	36 13	155	*LBLE	21 15
044	*LBL2	21 02	072	EEX	-23	100	6	06	128	1	01	156	STOC	35 13
045	STOA	35 11	073	3	03	101	+	-55	129	EEX	-23	157	R↓	-31
046	RCLi	36 45	074	×	-35	102	RCLA	36 11	130	3	03	158	STOB	35 12
047	FRC	16 44	075	FRC	16 44	103	RCLA	36 11	131	÷	-24	159	R↓	-31
048	1	01	076	1	01	104	X²	53	132	.	-62	160	STOA	35 11
049	EEX	-23	077	0	00	105	-	-45	133	0	00	161	2	02
050	3	03	078	0	00	106	.	-62	134	4	04	162	8	08
051	×	-35	079	×	-35	107	5	05	135	+	-55	163	STOD	35 14
052	INT	16 34	080	RCLE	36 15	108	6	06	136	PRTX	-14	164	R/S	51
053	1	01	081	×	-35	109	7	07	137	RCLD	36 14			
054	EEX	-23	082	RCLC	36 13	110	+	-55	138	×	-35			
055	3	03	083	X⇄Y	-41	111	÷	-24	139	.	-62			
056	÷	-24	084	F0?	16 23 00	112	PRTX	-14	140	0	00			

User instructions for HP version **Table VI**

Step	Procedure
1.	Store first 10 constants from Table III, numbers 08 to 17, in registers 0 to 9. Key **P⇆S**. Store next 10 constants, numbers 18 to 27, in secondary registers 0 to 9.
2.	Store these data on a data card: Key **WRITE DATA**.
3.	Store next 10 constants, numbers 28 to 37, in registers 0 to 9. Key **P⇆S**. Store next 5 constants, numbers 38 to 42, in secondary registers 0 to 4.
4.	Store these data on a second data card: Key **WRITE DATA**.

To run the program:

1a. Enter the program.

1b. Enter the first data card.

2. Enter the number and code for each structural group, following the nomenclature of Table I, with key **A**.
For example, for two $-CH_3$ groups, enter 2.08, key **A**
for three $-CH_2-$ groups, enter 3.09, key **A**
|
for two $-CH$ rings, enter 2.11, key **A**
|

3a. If structural groups beyond code 0.27 are not required, go to step 7.

3b. If structural groups beyond code 0.27 are required, use key **D**.

4. If structural groups beyond code 0.27 are required, enter second data card after key **D** of step 3b.

5. Use key **E** after having entered second data card. (The second data card wipes out the first data, but key **D** saves the calculation in the stack, which is not affected by data changes, and key **E** puts the calculation back in the calculator.)

6. Enter the balance of the data for structural groups beyond code 0.27, the same as step 2.

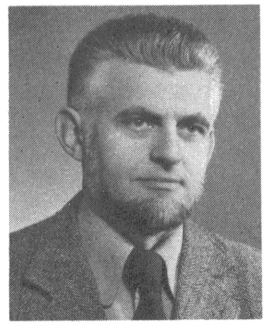
7. When all structural data are entered, enter molecular weight and boiling point, °C (*not* K)
Molecular weight — key **Enter ↑**
Boiling point, °C — key **B**

8. Output will be:
Critical temperature, K
Critical pressure, atm
Critical volume, L/g-mol
Critical compressibility factor

Notes: 1. If erroneous data are entered in steps 2 or 6, they may be deleted by reentering the same data with key **a**.
2. For *cis-* and *trans-* structures, with the same structural formulas, the molecular weights and different boiling points can be entered at step 7.

References

1. Lydersen, A. L., University of Wisconsin, College of Engineering, Engineering Experimental Station, Report 3, April 1955.
2. Hougen, O. A., et al., "Chemical Process Principles—Part I," 2nd ed., John Wiley & Sons, Inc., New York, 1954, p. 87.
3. Reid, R. C., et al., "The Properties of Gases and Liquids," 3rd ed., McGraw-Hill Book Co., New York, 1977, p. 12.
4. Fishtine, S. H., *Ind. Eng. Chem. Fundamentals,* 2, p. 1949 (1963).



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Predict thermal conductivities of gas mixtures and liquids

TI-59 programs calculate the thermal conductivities of binary gaseous mixtures and liquids over a range of temperatures and from a minimum amount of data.

James H. Weber, *University of Nebraska**

☐ For determining the thermal conductivities of gaseous mixtures, Wassiljewa postulated the general correlation [*1*]:

$$\lambda_m = \sum_{i=1}^{n} \left(\frac{y_i \lambda_i}{\sum_{j=1}^{n} y_1 A_{ij}} \right) \quad (1)$$

For a binary mixture:

$$\lambda_m = \frac{y_1 \lambda_1}{y_1 + A_{12} y_2} + \frac{y_2 \lambda_2}{y_2 + y_1 A_{21}} \quad (1a)$$

For the term A_{ij}, Lindsay and Bromley suggested [*2*]:

$$A_{12} = \frac{1}{4}\left\{1 + \left[\frac{\eta_1}{\eta_2}\left(\frac{M_2}{M_1}\right)^{3/4} \frac{T + S_1}{T + S_2}\right]^{1/2}\right\}^2 \frac{T + S_{12}}{T + S_1} \quad (2)$$

Here: $$S_1 = 1.5 T_{b_1} \quad (3)$$

and: $$S_{12} = S_{21} = C_s (S_1 S_2)^{1/2} \quad (4)$$

Eq. (1a) and (2) have been programmed assuming that M, η, T_b, S and λ are known for both components. The thermal conductivity of the mixture, λ_m, can be calculated by entering t(°C), pressing **A**, and then entering y_1 and pressing **R/S.** The value for λ_m, in cal/(cm)(s)(K) and Btu/(ft)(h)(°R), is calculated and printed. The temperature and mole fraction of Component 1 are also printed.

Viscosities and heat capacities computed

In many cases, all the data required for the foregoing calculation will not be readily available, so programs to calculate these are also included. To calculate T_b and S, first enter t_{b_1}(°C) and press the **B** key, then enter t_{b_2}(°C) and press **R/S.** In both cases, the normal boiling point, t(°C), is printed, and T_b and S are calculated and stored.

If the viscosities are unknown, these can be calculated via the Yoon-Thodos correlation [*3*] by entering t(°C) and pressing **C**:

$$\eta\xi = 4.610\, T_r^{0.618} - 2.04e^{-0.449\, T_r} + 1.94e^{-4.058\, T_r} + 0.1 \quad (5)$$

Values for η_1 and η_2 (in μP) are calculated, stored in the proper locations and printed, with η_2 also displayed. If a printer is not used, either the **PRT** command (Step **290**) may be eliminated or an **R/S** command substituted, depending on the wishes of the user.

Because heat capacities are usually required in the calculation of thermal conductivities, a program to calculate them is also included. To use it, enter t(°C) and press **E**, and values of C_p will be calculated via the relationship:

$$C_p = a + bT + cT^2 + dT^3 \quad (6)$$

Heat capacities are stored and printed. The value for C_{p_2} is displayed. The calculation may be stopped to display C_{p_1}, if an **R/S** command is substituted for the **PRT** command at Step **503**.

Component thermal conductivity

The necessary information is now available to calculate the thermal conductivity values for the two pure components by the relationship of Stiel and Thodos [*4*]:

$$\lambda M/\eta = 1.15 C_v + 4.04 \quad (7)$$

*For information about the author, see p. 77.

Originally published March 9, 1981.

Programs for calculating thermal conductivities of mixtures, S, viscosities, thermal conductivities of pure components, and heat capacities

Table I

Location	Code	Key
Calculate interaction coefficient by Lindsay-Bromley correlation		
000	76	LBL
001	16	A'
002	93	.
003	02	2
004	05	5
005	65	×
006	53	(
007	01	1
008	85	+
009	53	(
010	53	(
011	43	RCL
012	02	02
013	55	÷
014	43	RCL
015	03	03
016	54	)
017	42	STO
018	11	11
019	65	×
020	53	(
021	53	(
022	43	RCL
023	01	01
024	55	÷
025	43	RCL
026	00	00
027	54	)
028	45	Y^x
029	53	(
030	03	3
031	55	÷
032	04	4
033	54	)
034	54	)
035	42	STO
036	12	12
037	65	×
038	53	(
039	53	(
040	43	RCL
041	06	06
042	85	+
043	43	RCL
044	07	07
045	54	)
04D	55	÷
047	53	(
048	43	RCL
049	06	06
050	85	+
051	43	RCL
052	08	08
053	54	)
054	42	STO
055	15	15
056	54	)
057	42	STO
058	13	13
059	54	)
060	34	$\sqrt{X}$
061	54	)
062	33	X^2
063	65	×
064	53	(
065	53	(
066	43	RCL
067	06	06
068	85	+
069	53	(
070	43	RCL
071	09	09
072	65	×
073	53	(
074	43	RCL
075	07	07
076	65	×
077	43	RCL
078	08	08
079	54	)
080	34	$\sqrt{X}$
081	54	)
082	54	)
083	42	STO
084	14	14
085	55	÷
086	53	(
087	43	RCL
088	06	06
089	85	+
090	43	RCL
091	07	07
092	54	)
093	54	)
094	95	=
095	42	STO
096	10	10
097	93	.
098	02	2
099	05	5
100	65	×
101	53	(
102	01	1
103	85	+
104	53	(
105	53	(
106	43	RCL
107	11	11
108	35	1/X
109	54	)
110	65	×
111	53	(
112	43	RCL
113	12	12
114	35	1/X
115	54	)
116	65	×
117	53	(
118	43	RCL
119	13	13
120	35	1/X
121	54	)
122	54	)
123	34	$\sqrt{X}$
124	54	)
125	33	X^2
126	65	×
127	53	(
128	43	RCL
129	14	14
130	55	÷
131	43	RCL
132	15	15
133	54	)
134	95	=
135	42	STO
136	16	16
137	92	RTN
Calculate λ_m by Wassiljewa correlation		
Enter t(°C)		
138	76	LBL
139	11	A
140	99	PRT
141	85	+
142 ⅞	43	RCL
143	21	21
144	95	=
145	42	STO
146	06	06
147	91	R/S
Enter y_1		
148	99	PRT
149	42	STO
150	17	17
151	75	−
152	01	1
153	95	=
154	94	+/−
155	42	STO
156	18	18
157	16	A'
158	43	RCL
159	18	18
160	65	×
161	43	RCL
162	20	20
163	55	÷
164	53	(
165	43	RCL
166	18	18
167	85	+
168	53	(
169	43	RCL
170	16	16
171	65	×
172	43	RCL
173	17	17
174	54	)
175	54	)
176	85	+
177	53	(
178	53	(
179	43	RCL
180	17	17
181	65	×
182	43	RCL
183	19	19
184	54	)
185	55	÷
186	53	(
187	43	RCL
188	17	17
189	85	+
190	53	(
191	43	RCL
192	10	10
193	65	×
194	43	RCL
195	18	18
196	54	)
197	54	)
198	54	)
199	95	=
200	99	PRT
201	55	÷
202	43	RCL
203	48	48
204	95	=
205	99	PRT
206	91	R/S
Calculate T_b and S		
Enter t_{b_1} (°C)		
207	76	LBL
208	12	B
209	99	PRT
210	85	+
211	43	RCL
212	21	21
213	95	=
214	42	STO
215	04	04
216	65	×
217	01	1
218	93	.
219	05	5
220	95	=
221	42	STO
222	07	07
223	91	R/S
Enter t_{b_2} (°C)		
224	99	PRT
225	85	+
226	43	RCL
227	21	21
228	95	=
229	42	STO
230	05	05
231	65	×
232	01	1
233	93	.
234	05	5
235	95	=
236	42	STO
237	08	08
238	91	R/S
Calculate viscosities by Yoon-Thodos correlation		
Enter t(°C)		
239	76	LBL
240	13	C
241	99	PRT
242	42	STO
243	33	33
244	85	+
245	43	RCL
246	21	21
247	95	=
248	55	÷
249	43	RCL
250	22	22
251	95	=
252	42	STO
253	32	32
254	71	SBR
255	38	SIN
256	55	÷
257	53	(
258	53	(
259	43	RCL
260	22	22
261	45	Y^x
262	53	(
263	01	1
264	55	÷
265	06	6
266	54	)
267	54	)
268	55	÷
269	53	(
270	53	(
271	43	RCL
272	00	00
273	34	$\sqrt{X}$
274	54	)
275	65	×
276	53	(
277	43	RCL
278	23	23
279	45	Y^x
280	53	(
281	02	2
282	55	÷
283	03	3
284	54	)
285	54	)
286	54	)
287	95	=
288	42	STO
289	02	02
290	99	PRT
291	43	RCL
292	33	33
293	85	+
294	43	RCL
295	21	21
296	95	=
297	55	÷
298	43	RCL
299	24	24
300	95	=
301	42	STO
302	32	32
303	71	SBR
304	38	SIN
305	55	÷
306	53	(
307	53	(
308	43	RCL
309	24	24
310	45	Y^x
311	53	(
312	01	1
313	55	÷
314	06	6
315	54	)
316	54	)
317	55	÷
318	53	(
319	53	(
320	43	RCL
321	01	01
322	34	$\sqrt{X}$
323	54	)
324	65	×
325	53	(
326	43	RCL
327	25	25
328	45	Y^x
329	53	(
330	02	2
331	55	÷
332	03	3
333	54	)
334	54	)
335	54	)
336	95	=
337	42	STO
338	03	03
339	99	PRT
340	91	R/S
Subroutine		
341	76	LBL
342	38	SIN
343	53	(
344	53	(
345	43	RCL
346	26	26
347	65	×
348	43	RCL
349	32	32
350	45	Y^x
351	53	(
352	43	RCL
353	27	27
354	54	)
355	54	)
356	75	−
357	53	(
358	43	RCL
359	30	30
360	65	×
361	53	(
362	53	(
363	43	RCL
364	28	28
365	65	×
366	43	RCL
367	32	32
368	54	)
369	22	INV
370	23	LNX
371	54	)
372	54	)
373	85	+

(Continued) Table I

Location	Code	Key
374	53	(
375	43	RCL
376	31	31
377	65	×
378	53	(
379	53	(
380	43	RCL
381	29	29
382	65	×
383	43	RCL
384	32	32
385	54	)
386	22	INV
387	23	LNX
388	54	)
389	54	)
390	85	+
391	93	•
392	01	1
393	54	)
394	92	RTN
Calculate λ by Stiel-Thodos correlation		
395	76	LBL
396	14	D
397	53	(

Location	Code	Key
398	53	(
399	43	RCL
400	34	34
401	75	−
402	43	RCL
403	36	36
404	54	)
405	65	×
406	43	RCL
407	37	37
408	85	+
409	43	RCL
410	38	38
411	54	)
412	65	×
413	53	(
414	53	(
415	43	RCL
416	39	39
417	65	×
418	43	RCL
419	02	02
420	54	)
421	55	÷
422	43	RCL
423	00	00
424	54	)
425	95	=
426	42	STO

Location	Code	Key
427	19	19
428	99	PRT
429	53	(
430	53	(
431	43	RCL
432	35	35
433	75	−
434	43	RCL
435	36	36
436	54	)
437	65	×
438	43	RCL
439	37	37
440	85	+
441	43	RCL
442	38	38
443	54	)
444	65	×
445	53	(
446	53	(
447	43	RCL
448	39	39
449	65	×
450	43	RCL
451	03	03
452	54	)
453	55	÷
454	43	RCL
455	01	01

Location	Code	Key
456	54	)
457	95	=
458	42	STO
459	20	20
460	99	PRT
461	91	R/S
Calculate C_p Enter t(°C)		
462	76	LBL
463	15	E
464	99	PRT
465	85	+
466	43	RCL
467	21	21
468	95	=
469	42	STO
470	06	06
471	43	RCL
472	40	40
473	85	+
474	53	(
475	43	RCL
476	41	41
477	65	+
478	43	RCL
479	06	06
480	54	)

Location	Code	Key
481	85	+
482	53	(
483	43	RCL
484	06	06
485	33	X^2
486	65	×
487	43	RCL
488	42	42
489	54	)
490	85	+
491	53	(
492	43	RCL
493	06	06
494	45	Y^x
495	03	3
496	65	×
497	43	RCL
498	43	43
499	54	)
500	95	=
501	42	STO
502	34	34
503	99	PRT
504	43	RCL
505	44	44
506	85	+
507	53	(
508	43	RCL
509	45	45

Location	Code	Key
510	65	×
511	43	RCL
512	06	06
513	54	)
514	85	+
515	53	(
516	43	RCL
517	06	06
518	33	X^2
519	65	×
520	43	RCL
521	46	46
522	54	)
523	85	+
524	53	(
525	43	RCL
526	06	06
527	45	Y^x
528	03	3
529	65	×
530	43	RCL
531	47	47
532	54	)
533	95	=
534	42	STO
535	35	35
536	99	PRT
537	91	R/S

Nomenclature

A Constant of Eq. (9)
A_{ij} Interaction coefficient, defined by Eq. (2)
a, b, c, d Constants of Eq. (6)
C_p Heat capacity at constant pressure, cal/(g-mol)(°C)
C_v Heat capacity at constant volume, cal/(g-mol)(°C)
C_s Constant of Eq. (4)
M Molecular weight
N' Number of atoms in molecule of a substance
P Pressure, atm
R Gas law constant, 1.987 cal/(g-mol)(K) or 82.07 (cm³)(atm)(g-mol)(K)
S Constant, defined by Eq. (3), K
T Temperature, K
t Temperature, °C
y Vapor-phase mole fraction
Z Compressibility factor
ξ $T_c^{1/6}/M^{1/2}P_c^{2/3}$
η Viscosity, μP
λ Thermal conductivity, cal/(cm)(s)(K) or Btu/(ft)(h)(°R)
ρ Density, g-mol/cm³
ω Pitzer's acentric factor

Superscripts

o Ideal gas state

Subscripts

b Normal boiling point
c Critical
i,j Refers to components in mixtures
L Liquid
r Reduced
s Saturated
0 0°C
1,2 Components 1 and 2 of a binary mixture

By pressing **D**, values for λ will be calculated, printed and stored in the proper locations, and λ_2 displayed. The calculation can be stopped in order to display λ_1 if an **R/S** command is substituted for **PRT** at Step **428.**

The inclusion of programs for calculating S, η, C_p and λ of two pure components permits computation of thermal conductivities of mixtures from a minimum amount of data. If all, or part, of the fundamental data is available, this can be placed in the proper storage locations, with uncertainties correspondingly reduced.

The programs that have been discussed are given in Table I and the storage information in Table II. The programs and storage require both channels of two magnetic cards. The partitioning is 559.49.

For comparison, thermal conductivities of a gaseous mixture of 39.4 mol% methane with *n*-butane have been calculated, and these are compared in Table III with experimental data reported by Carmichael, Jacobs and Sage [5]. It should be noted that the calculated values were determined from a minimum amount of fundamental data.

Thermal conductivities of liquids

There are a number of correlations for predicting the thermal conductivities of liquids. Two have been programmed. Both require the calculation of thermal conductivity at a relatively low temperature, after which values at higher temperatures are calculated by taking into account the effect of temperature.

The first correlation is that of Sato [*6*]:

$$\lambda_{Lb} = (2.64 \times 10^{-3})/M^{1/2} \qquad (8)$$

Riedel suggested the relationship [*7,8*]:

$$\lambda_L = A[1 + (20/3)(1 - T_r)^{2/3}] \qquad (9)$$

Eq. (8) and (9) yield:

$$\lambda_L = \left[\frac{2.64 \times 10^{-3}}{M^{1/2}}\right]\left[\frac{3 + 20(1 - T_r)^{2/3}}{3 + 20(1 - T_{rb})^{2/3}}\right] \qquad (10)$$

These permit the calculation of thermal conductivity values at temperatures other than the normal boiling point from a minimum amount of data.

To determine λ_L values via Eq. (8) and (10), enter t_b(°C) and press **A**, then enter t(°C) and press **R/S,** and λ_{Lb} will be calculated and printed.

The calculations are not stopped, and the thermal conductivity at temperature t is calculated, displayed and printed. The two temperatures are also printed. Values of λ, in cal/(cm)(s)(K) and Btu/(ft)(h)(°R), are printed. If a printer is not used, the value of λ_{Lb}, if it is desired, is stored at Location **11.** Also, the program can be stopped by an **R/S** command, in place of **PRT,** in Step **13,** and the λ_{Lb} value will then be displayed.

The programs for Eq. (8) and (10) are given in Table IV, and the storage information in Table V. Calculated results for *n*-butane are compared in Table VI to experimental values reported by Carmichael and Sage [*14*].

Second correlation for liquids

Missenard proposed the relationship [*9,10*]:

$$\lambda_{Lo} = \frac{84 \times 10^{-6}(T_b\rho_o)^{1/2}C_{p_{Lo}}}{M^{1/2}N'^{1/4}} \qquad (11)$$

In Eq. (11), λ_{Lo} is the thermal conductivity at 0°C.

Combining Eq. (11) with Eq. (9) gives:

$$\lambda_L = \lambda_{Lo}\left\{\frac{3 + 20(1 - T_r)^{2/3}}{3 + 20[1 - (273/T_c)]^{2/3}}\right\} \qquad (12)$$

Eq. (11) and (12) have been programmed. To determine λ values via them, enter t_b(°C) and press **B**, and follow by entering t(°C) and pressing **R/S.** After λ_{Lo} is calculated and printed, λ_L is calculated, displayed and printed.

To stop the calculations so as to display λ_{Lo}, substitute **R/S** for **PRT** at Location **118.** If the two temperatures are already in place, as would be the case if calculations using Eq. (8) and (10) had been made, the temperatures need not be reentered, but only **B** pressed, and the calculation proceeds as has already been outlined.

The programs for Eq. (11) and (12) are listed in Table IV, and the storage information in Table V.

Calculated results for *n*-butane are compared in Table VI to experimental values reported by Carmichael and Sage [*14*]. In these calculations, values for ρ_o, C_p^o and C_{p_o} are computed by methods that will be discussed.

To use Eq. (11) and (12), liquid density and heat capacity at 0°C must be known. If these values are available, they can be stored in locations **13** and **14.** If

Storage information for the calculation of thermal conductivities of gaseous mixtures — Table II

00	M_1	25	P_{c_2}	
01	M_2	26	4.61	Constants of Eq. (5)
02	η_1†	27	0.618	
03	η_2†	28	−0.449	
04	T_{b_1}†	29	−4.058	
05	T_{b_2}†	30	2.04	
06	T*	31	1.94	
07	S_1†	32	T_{r_1}* or T_{r_2}*	
08	S_2†	33	t°C	
09	C_S‡	34	C_{p_1}†	
10	A_{12}*	35	C_{p_2}†	
11	η_1/η_2*	36	$R = 1.987$	cal/(g-mol) (K)
12	$(M_2/M_1)^{3/4}$*	37	1.15	Constants of Eq. (7)
13	$(T+S_1)/(T+S_2)$*	38	4.04	
14	$(T+S_{12})$*	39	0.000001	
15	$(T+S_2)$*	40	a	Constants of C_p expression, Component 1
16	A_{21}*	41	b	
17	y_1	42	c	
18	y_2*	43	d	
19	λ_1†	44	a	Constants of C_p expression, Component 2
20	λ_2†	45	b	
21	273.16	46	c	
22	T_{c_1}	43	d	
23	P_{c_1}	48	0.004134	Conversion factor for λ values
24	T_{c_2}			

* Calculated and stored by program
† Either entered or calculated
‡ Constant of Eq. (4); usually equals 1, but can be changed by user.

Calculated and experimental conductivities for 39.4% mixture of methane with *n*-butane — Table III

t, °C	$\lambda \times 10^6$, cal/(cm)(s)(K)	
(P=1 atm)	Ref. [5]	Eq. (1), (2)*
4.44	48.8	42.8
37.73	54.2	50.3
71.11	61.6	59.0
104.4	70.7	68.0
137.8	80.2	77.6
171.1	90.5	87.5

* Values for η and C_p were calculated from empirical relationships.

Programs for calculating liquid-phase thermal conductivities by the correlations of Sato, Riedel and Missenard, and for calculating liquid density, and liquid and gas heat-capacities — Table IV

Calculate λ_L by Sato and Riedel correlations

Enter t_b(°C) t(°C)

Location	Code	Key
000	76	LBL
001	11	A
002	71	SBR
003	48	EXC
004	53	(
005	43	RCL
006	08	08
007	65	×
008	43	RCL
009	09	09
010	54	)
011	55	÷
012	43	RCL
013	02	02
014	34	$\sqrt{X}$
015	95	=
016	42	STO
017	11	11
018	99	PRT
019	55	÷
020	43	RCL
021	29	29
022	95	=
023	99	PRT
024	43	RCL
025	11	11
026	71	SBR
027	38	SIN
028	95	=
029	99	PRT
030	55	÷
031	43	RCL
032	29	29
033	95	=
034	99	PRT
035	91	R/S

Subroutine

Location	Code	Key
036	76	LBL
037	38	SIN
038	65	×
039	53	(
040	53	(
041	03	3
042	85	+
043	02	2
044	00	0
045	65	×
046	53	(
047	01	1
048	75	−
049	43	RCL
050	10	10
051	54	)
052	45	Y^x
053	53	(
054	02	2
055	55	÷
056	03	3
057	54	)
058	54	)
059	55	÷
060	53	(
061	03	3
062	85	+
063	02	2
064	00	0
065	65	×
066	53	(
067	01	1
068	75	÷
069	53	(
070	43	RCL
071	06	06
072	55	÷
073	43	RCL
074	00	00
075	54	)
076	54	)
077	45	Y^x
078	53	(
079	02	2
080	55	÷
081	03	3
082	54	)
083	54	)
084	54	)
085	92	RTN

Calculate λ_L by Missenard and Riedel correlations

Enter t_b(°C) t°C

Location	Code	Key
086	76	LBL
087	17	B'
088	71	SBR
089	48	EXC
090	76	LBL
091	12	B
092	53	(
093	53	(
094	08	8
095	04	4
096	65	×
097	43	RCL
098	12	12
099	65	×
100	53	(
101	43	RCL
102	06	06
103	65	×
104	43	RCL
105	13	13
106	54	)
107	34	$\sqrt{X}$
108	65	×
109	43	RCL
110	14	14
111	54	)
112	55	÷
113	53	(
114	43	RCL
115	02	02
116	34	$\sqrt{X}$
117	65	×
118	43	RCL
119	05	05
120	45	Y^x
121	53	(
122	01	1
123	55	÷
124	04	4
125	54	)
126	54	)
127	54	)
128	42	STO
129	11	11
130	99	PRT
131	55	÷
132	43	RCL
133	29	29
134	95	=
135	99	PRT
136	43	RCL
137	06	06
138	42	STO
139	15	15
140	43	RCL
141	07	07
142	42	STO
143	06	06
144	43	RCL
145	11	11
146	71	SBR
147	38	SIN
148	95	=
149	99	PRT
150	55	÷
151	43	RCL
152	29	29
153	95	=
154	99	PRT
155	42	STO
156	28	28
157	43	RCL
158	15	15
159	42	STO
160	06	06
161	43	RCL
162	28	28
163	91	R/S

Subroutine

Location	Code	Key
164	76	LBL
165	48	EXC
166	99	PRT
167	85	+
168	43	RCL
169	07	07
170	95	=
171	42	STO
172	06	06
173	91	R/S
174	99	PRT
175	85	+
176	43	RCL
177	07	07
178	95	=
179	55	÷
180	43	RCL
181	00	00
182	95	=
183	42	STO
184	10	10
185	92	RTN

Calculate ideal gas phase $C_p(C_p°)$

Enter t(°C)

Location	Code	Key
186	76	LBL
187	18	C'
188	99	PRT
189	85	+
190	43	RCL
191	07	07
192	95	=
193	65	×
194	43	RCL
195	17	17
196	85	+
197	43	RCL
198	16	16
199	85	+
200	53	(
201	43	RCL
202	07	07
203	33	X^2
204	65	×
205	43	RCL
206	18	18
207	54	)
208	85	+
209	53	(
210	43	RCL
211	07	07
212	45	Y^x
213	03	3
214	65	×
215	43	RCL
216	19	19
217	54	)
218	95	=
219	99	PRT
220	42	STO
221	25	25
222	91	R/S

Calculate liquid phase $C_p(C_{pL})$

Enter t(°C)

Location	Code	Key
223	76	LBL
224	13	C
225	71	SBR
226	58	FIX
227	53	(
228	43	RCL
229	20	20
230	85	+
231	53	(
232	43	RCL
233	21	21
234	65	×
235	53	(
236	01	1
237	75	−
238	43	RCL
239	10	10
240	54	)
241	35	1/X
242	54	)
243	85	+
244	53	(
245	43	RCL
246	03	03
247	65	×
248	53	(
249	43	RCL
250	22	22
251	85	+
252	53	(
253	43	RCL
254	23	23
255	65	×
256	53	(
257	01	1
258	75	−
259	43	RCL
260	10	10
261	54	)
262	45	Y^x
263	53	(
264	01	1
265	55	÷
266	03	3
267	54	)
268	65	×
269	43	RCL
270	10	10
271	35	1/X
272	54	)
273	85	+
274	53	(
275	43	RCL
276	24	24
277	65	×
278	53	(
279	01	1
280	75	−
281	43	RCL
282	10	10
283	54	)
284	35	1/X
285	54	)
286	54	)
287	54	)
288	54	)
289	65	×
290	43	RCL
291	04	04
292	85	+
293	43	RCL
294	25	25
295	95	=
296	99	PRT
297	42	STO
298	14	14
299	91	R/S

Calculate liquid density

Enter t(°C)

Location	Code	Key
300	76	LBL
301	14	D
302	53	(
303	53	(
304	43	RCL
305	27	27
306	65	×
307	43	RCL
308	00	00
309	54	)
310	55	÷
311	43	RCL
312	01	01
313	54	)
314	65	×
315	53	(
316	43	RCL
317	26	26
318	45	Y^x
319	53	(
320	01	1
321	85	+
322	53	(
323	01	1
324	75	−
325	43	RCL
326	10	10
327	54	)
328	45	Y^x
329	53	(
330	02	2
331	55	÷
332	07	7
333	54	)
334	54	)
335	54	)
336	95	=
337	35	1/X
338	42	STO
339	13	13
340	99	PRT
341	91	R/S
342	76	LBL
343	19	D'
344	71	SBR
345	58	FIX
346	14	D

Subroutine

Location	Code	Key
347	76	LBL
348	58	FIX
349	99	PRT
350	85	+
351	43	RCL
352	07	07
353	95	=
354	55	÷
355	43	RCL
356	00	00
357	95	=
358	42	STO
359	10	10
360	92	RTN

Storage information for calculating conductivities of liquids, heat capacities and liquid densities **Table V**

00	T_c, K	15	T_b*	
01	P_c, atm	16	a	Constants of Eq. (6)
02	M	17	b	
03	ω	18	c	
04	R, 1.987	19	d	
05	N'	20	2.56	Constants of Eq. (12)
06	T_b*	21	0.436	
07	273.16 (0°C)	22	2.91	
08	2.64 Constant of Eq. (8)	23	4.28	
09	0.001	24	0.296	
10	T_r*	25	C_p°†	
11	λ_{Lb}*	26	Z_{RA}	
12	0.000001	27	R, 82.07	
13	ρ†	28	λ_L	
14	C_{pL}†			

* Quantities calculated and stored by program
† Quantities may be calculated or supplied by user

Calculated and experiment values of the thermal conductivities of liquid *n* butane **Table VI**

t, °C	λ*, Btu/(ft)(h)(°R)		
	Sato and Riedel	Missenard and Riedel	Carmichael and Sage
4.44	0.08237	0.07412	0.06340
37.73	0.07247	0.06521	0.05531
71.1	0.06152	0.05536	0.04819
104.4	0.04892	0.04402	0.04261
137.8	0.03248	0.02923	0.03609

* At bubble point

they are not, programs have been included to calculate them.

Calculate density and heat capacity

Density, ρ_o, can be calculated with the Rackett correlation as modified by Spencer and Danner [*11*]:

$$1/\rho_s = (RT_c/P_c)Z_{RA}^{[1+(1-T_r)^{2/7}]} \qquad (13)$$

To use the program to calculate Eq. (13), enter t(°C) and press **D**, whereupon ρ_s, in g-mol/cm^3, will be calculated, printed and stored in Location **13.** If the temperature is already in place as a result of a previous calculation, press **D** and the calculation will proceed. (In reality, saturated density is calculated, but the effect of pressure is negligible.)

Liquid heat capacity at 0°C may be calculated by the Rowlinson relationship [*12*] as modified by Bondi [*13*]:

$$(C_{p_L} - C_p^o)/R = 2.56 + 0.436(1 - T_r)^{-1} + \omega[2.91 + 4.28(1 - T_r)^{1/3}T_r^{-1} + 0.296(1 - T_r)^{-1}] \qquad (14)$$

If the gaseous heat-capacity datum is available, it should be stored at Location **25.** If the value must be calculated, the empirical constants required to use Eq. (6) must be stored, then t(°C) entered and **C′** pressed. The heat capacity in the ideal gas state is calculated, displayed, printed and stored at Location **25.** The liquid heat capacity can then be calculated by means of Eq. (14). Enter t(°C) and 0°C and press **C**, and $C_{p_{Lo}}$ will be stored at Location **14,** displayed and printed.

The programs for calculating ρ, C_p^o and C_{p_L} are given in Table IV, and the storage information in Table V.

The programs for calculating liquid thermal conductivity, liquid density, and heat capacities takes both channels of a magnetic card, and the storage requires one channel of another card. Partitioning is normal.

For HP-67/97 users

The HP version closely follows the TI programs. Tables VII and VIII offer listings for program A (for gas mixtures), and user instructions are given in Table IX. The program listing for liquid mixtures (program B) is contained in Table X, and user instructions in Table XI.

Listing for HP version—program A, part 1 (gas mixtures) **Table VII**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	020	R/S	51	039	GSB7	23 07	058	×	-35	077	5	05
002	2	02	021	*LBL2	21 02	040	*LBL3	21 03	059	STO5	35 05	078	×	-35
003	7	07	022	STO0	35 00	041	R/S	51	060	P⇄S	16-51	079	4	04
004	3	03	023	R/S	51	042	STO5	35 05	061	F0?	16 23 00	080	.	-62
005	.	-62	024	STO1	35 01	043	R↓	-31	062	GTO1	22 01	081	0	00
006	1	01	025	GTO3	22 03	044	STO4	35 04	063	SF0	16 21 00	082	4	04
007	6	06	026	*LBLE	21 15	045	P⇄S	16-51	064	R/S	51	083	+	-55
008	STOE	35 15	027	GSB9	23 09	046	F0?	16 23 00	065	GTO2	22 02	084	RCL2	36 02
009	+	-55	028	*LBL3	21 03	047	GTO1	22 01	066	*LBL7	21 07	085	×	-35
010	STOA	35 11	029	R/S	51	048	SF0	16 21 00	067	RCL1	36 01	086	RCL0	36 00
011	R↓	-31	030	STO2	35 02	049	P⇄S	16-51	068	1	01	087	÷	-24
012	STO3	35 03	031	GTO3	22 03	050	R/S	51	069	.	-62	088	STO3	35 03
013	CHS	-22	032	*LBLC	21 13	051	*LBLB	21 12	070	9	09	089	RTN	24
014	1	01	033	GSB2	23 02	052	STO4	35 04	071	8	08	090	*LBL9	21 09
015	+	-55	034	*LBL3	21 03	053	RCLE	36 15	072	6	06	091	P⇄S	16-51
016	P⇄S	16-51	035	R/S	51	054	+	-55	073	-	-45	092	STOI	35 46
017	STO9	35 09	036	STO3	35 03	055	1	01	074	1	01	093	R↓	-31
018	P⇄S	16-51	037	GTO3	22 03	056	.	-62	075	.	-62	094	RCLA	36 11
019	CF0	16 22 00	038	*LBLD	21 14	057	5	05	076	1	01	095	×	-35

(Continued) Table VII

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
096	+	-55	122	Yˣ	31	148	0	00	174	RCL5	36 05	200	+	-55
097	RCLA	36 11	123	÷	-24	149	4	04	175	P⇄S	16-51	201	÷	-24
098	×	-35	124	RCLA	36 11	150	×	-35	176	RCL5	36 05	202	×	-35
099	+	-55	125	RCLI	36 46	151	−	-45	177	×	-35	203	√X	54
100	RCLA	36 11	126	÷	-24	152	4	04	178	P⇄S	16-51	204	1/X	52
101	×	35	127	STOI	35 46	153	.	-62	179	√X	54	205	STO6	35 06
102	RCLI	36 46	128	.	-62	154	0	00	180	STOB	35 12	206	P⇄S	16-51
103	+	-55	129	6	06	155	5	05	181	RCL2	36 02	207	1/X	52
104	STO1	35 01	130	1	01	156	8	08	182	P⇄S	16-51	208	1	01
105	RTN	24	131	8	08	157	RCLI	36 46	183	RCL2	36 02	209	+	-55
106	*LBL3	21 03	132	Yˣ	31	158	×	-35	184	÷	-24	210	X²	53
107	STOI	35 46	133	4	04	159	CHS	-22	185	RCL8	36 08	211	4	04
108	R↓	-31	134	.	-62	160	eˣ	33	186	P⇄S	16-51	212	÷	-24
109	2	02	135	5	05	161	1	01	187	RCL0	36 00	213	RCLA	36 11
110	ENT↑	-21	136	1	01	162	.	-62	188	÷	-24	214	RCLB	36 12
111	3	03	137	×	-35	163	9	09	189	.	-62	215	+	-55
112	÷	-24	138	RCLI	36 46	164	4	04	190	7	07	216	×	-35
113	Yˣ	31	139	.	-62	165	×	-35	191	5	05	217	RCLA	36 11
114	RCL8	36 08	140	4	04	166	+	-55	192	Yˣ	31	218	RCL5	36 05
115	√X	54	141	4	04	167	.	-62	193	×	-35	219	+	-55
116	×	-35	142	9	09	168	1	01	194	RCLA	36 11	220	÷	-24
117	RCLI	36 46	143	×	-35	169	+	-55	195	RCL5	36 05	221	STO7	35 07
118	1	01	144	CHS	-22	170	×	-35	196	+	-55	222	R/S	51
119	ENT↑	-21	145	eˣ	33	171	STO2	35 02	197	RCLA	36 11			
120	6	06	146	2	02	172	RTN	24	198	P⇄S	16-51			
121	÷	-24	147	.	-62	173	*LBL1	21 01	199	RCL5	36 05			

Listing for HP version—program A, part 2 (gas mixtures) **Table VIII**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	011	RCLB	36 12	021	P⇄S	16-51	031	1	01	041	RCL9	36 09
002	P⇄S	16-51	012	+	-55	022	GSB1	23 01	032	3	03	042	RCL7	36 07
003	RCL6	36 06	013	×	-35	023	+	-55	033	4	04	043	P⇄S	16-51
004	1	01	014	RCLA	36 11	024	PRTX	-14	034	÷	-24	044	RCL9	36 09
005	+	-55	015	RCL5	36 05	025	CF0	16 22 00	035	PRTX	-14	045	×	-35
006	X²	53	016	+	-55	026	P⇄S	16-51	036	R/S	51	046	+	-55
007	4	04	017	÷	-24	027	.	-62	037	*LBL1	21 01	047	÷	-24
008	÷	-24	018	STO7	35 07	028	0	00	038	RCL9	36 09	048	RTN	24
009	RCL8	36 08	019	P⇄S	16-51	029	0	00	039	RCL3	36 03	049	R/S	51
010	RCLA	36 11	020	GSB1	23 01	030	4	04	040	×	-35			

User instructions for HP version—program A (gas mixtures) **Table IX**

Part 1. Insert program card for Part 1.

Enter mole fraction of first component	**ENTER ↑**
Enter temperature, °C	Key **A**
For each component enter:	
1. Molecular weight	Key **R/S**
2. Heat capacity, cal/(g-mol)(°C), or Constants of Eq. 6.	Key **R/S,** or a **ENTER ↑**, b **ENTER ↑**, c **ENTER ↑**, d Key **E**
3. Viscosity, μP, or Critical pressure, atm, and temperature, K, for calculation of Eq. 5.	Key **R/S,** or P_c **ENTER ↑**, T_c Key **C**
4. Thermal conductivity of gas, cal/(cm)(s)(K), or No input and press for calculation of Eq. 7.	Key **R/S,** or Key **D**

(Continued) Table IX

5. Boiling temperature, °C, and S (from Eq. 3), or Boiling temperature, °C, for calculation of Eq. 3.	**ENTER ↑** Key **R/S**, or Key **B**

6. Return to step 1 with data for second component

(Note: If an incorrect input is made at any point, please start again from the beginning with mole fraction of first component, etc.)

Part 2. When program stops, insert program card for Part 2, and press key **A.**

Output will be thermal conductivity of the mixture,
first in cal/(cm)(s)(K), and
then in Btu/(ft)(h)(R).

Registers will have the following data (primary registers for first component and secondary registers for second component):

Molecular weight	Register 0
Heat capacity	Register 1
Viscosity	Register 2
Thermal conductivity	Register 3
Boiling point, °C	Register 4
S value (Eq. 3), K	Register 5

Listing for HP version—program B (liquid mixtures) **Table X**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	044	÷	-24	087	RCL6	36 06	130	+	-55	173	6	06
002	GSB0	23 00	045	-	-45	088	STOD	35 14	131	STO8	35 08	174	+	-55
003	2	02	046	2	02	089	RCL7	36 07	132	P⇄S	16-51	175	P⇄S	16-51
004	.	-62	047	ENT↑	-21	090	STO6	35 06	133	PRTX	-14	176	RCL4	36 04
005	6	06	048	3	03	091	RCL9	36 09	134	SPC	16-11	177	×	-35
006	4	04	049	÷	-24	092	GSB1	23 01	135	R/S	51	178	P⇄S	16-51
007	EEX	-23	050	Y^x	31	093	PRTX	-14	136	*LBLC	21 13	179	RCL8	36 08
008	CHS	-22	051	2	02	094	RCLA	36 11	137	GSB2	23 02	180	+	-55
009	3	03	052	0	00	095	÷	-24	138	P⇄S	16-51	181	PRTX	-14
010	RCL2	36 02	053	×	-35	096	PRTX	-14	139	1	01	182	STOC	35 13
011	√X	54	054	3	03	097	STOI	35 46	140	RCLB	36 12	183	SPC	16-11
012	÷	-24	055	+	-55	098	RCLD	36 14	141	-	-45	184	P⇄S	16-51
013	STO9	35 09	056	÷	-24	099	STO6	35 06	142	1	01	185	R/S	51
014	PRTX	-14	057	RTN	24	100	RCLI	36 46	143	ENT↑	-21	186	*LBLD	21 14
015	RCLA	36 11	058	*LBLB	21 12	101	R/S	51	144	3	03	187	GSB2	23 02
016	÷	-24	059	GSB0	23 00	102	*LBL0	21 00	145	÷	-24	188	P⇄S	16-51
017	PRTX	-14	060	8	08	103	RCL7	36 07	146	Y^x	31	189	RCL9	36 09
018	SPC	16-11	061	4	04	104	+	-55	147	RCL6	36 06	190	1	01
019	RCL9	36 09	062	EEX	-23	105	STO6	35 06	148	×	-35	191	RCLB	36 12
020	GSB1	23 01	063	6	06	106	R/S	51	149	RCLB	36 12	192	-	-45
021	PRTX	-14	064	CHS	-22	107	*LBL2	21 02	150	1/X	52	193	2	02
022	RCLA	36 11	065	RCL6	36 06	108	RCL7	36 07	151	×	-35	194	ENT↑	-21
023	÷	-24	066	RCL8	36 08	109	+	-55	152	RCL7	36 07	195	7	07
024	PRTX	-14	067	×	-35	110	RCL0	36 00	153	1	01	196	÷	-24
025	R/S	51	068	√X	54	111	÷	-24	154	RCLB	36 12	197	Y^x	31
026	*LBL1	21 01	069	×	-35	112	STOB	35 12	155	-	-45	198	1	01
027	1	01	070	RCLC	36 13	113	RTN	24	156	÷	-24	199	+	-55
028	RCLB	36 12	071	×	-35	114	*LBLc	21 16 13	157	+	-55	200	Y^x	31
029	-	-45	072	RCL2	36 02	115	RCL7	36 07	158	RCL5	36 05	201	P⇄S	16-51
030	2	02	073	√X	54	116	+	-55	159	+	-55	202	RCL0	36 00
031	ENT↑	-21	074	÷	-24	117	STOI	35 46	160	P⇄S	16-51	203	×	-35
032	3	03	075	RCL5	36 05	118	P⇄S	16-51	161	RCL3	36 03	204	RCL1	36 01
033	÷	-24	076	.	-62	119	RCL3	36 03	162	×	-35	205	÷	-24
034	Y^x	31	077	2	02	120	×	-35	163	P⇄S	16-51	206	RCLE	36 15
035	2	02	078	5	05	121	RCL2	36 02	164	RCL4	36 04	207	×	-35
036	0	00	079	Y^x	31	122	+	-55	165	1	01	208	1/X	52
037	×	-35	080	÷	-24	123	RCLI	36 46	166	RCLB	36 12	209	STO8	35 08
038	3	03	081	STO9	35 09	124	×	-35	167	-	-45	210	PRTX	-14
039	+	-55	082	PRTX	-14	125	RCL1	36 01	168	÷	-24	211	SPC	16-11
040	×	-35	083	RCLA	36 11	126	+	-55	169	+	-55	212	RTN	24
041	1	01	084	÷	-24	127	RCLI	36 46	170	2	02	213	R/S	51
042	RCL6	36 06	085	PRTX	-14	128	×	-35	171	.	-62			
043	RCL0	36 00	086	SPC	16-11	129	RCL0	36 00	172	5	05			

User instructions for HP version—program B (liquid mixtures) **Table XI**

For Sato-Riedel correlation:

Store the following data:	
Critical temperature, K, T_c	Register 0
Molecular weight, M	Register 2
Constant, 273.16	Register 7
Constant, 0.004134	Register **A**
Enter boiling point, °C, t_b	Key **A**
Enter temperature, °C, t	Key **R/S**

Output is thermal conductivity:
of liquid at boiling point, cal/(cm)(s)(K) and Btu/(ft)(h)(R)
of liquid at temperature, cal/(cm)(s)(K) and Btu/(ft)(h)(R)

For Missenard correlation:

Store same data as above plus the following:	
Constant, 1.987	Register 4
Number of atoms in molecule, N'	Register 5
Density, g-mol/cm^3, ρ	Register 8
(If density is not available, store the following:	
Critical pressure, atm, P_c	Register 1
Compressibility, Z_{RA}	Secondary register 9
Constant, 82.07	Register **E**
Enter temperature, °C	Key **D**)
Liquid heat capacity, C_{pL}, cal/(g-mol)(°C)	Register **C**
(If C_{pL} is not available, store the following:	
Ideal gas heat capacity, C_p°	Secondary register 8
Constant, 0.436	Secondary register 4
Constant, 2.91	Secondary register 5
Constant, 4.28	Secondary register 6
Constant, 0.296	Secondary register 7
Acentric factor, ω	Register 3
Enter temperature, °C	Key **C**)
(If C_p° is not available, store constants from Eq. 6:	
a	Secondary register 0
b	Secondary register 1
c	Secondary register 2
d	Secondary register 3
Enter temperature, °C	Key **c**)
Enter boiling point, °C, t_b	Key **B**
Enter temperature, °C, t	Key **R/S**

Output will be the same as for Sato-Riedel correlation.

If any of the parameters are calculated, their values will be printed at the end of the individual calculation.

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Predict thermal conductivities of liquid mixtures

Via programs for the TI-59, thermal conductivities of binary liquid mixtures can be calculated from the thermal conductivities of the pure components and the composition of the mixtures.

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☐ The thermal conductivities of binary liquid mixtures can be predicted with the Li correlation [1]:

$$\lambda_m = \Sigma\Sigma\ \phi_i \phi_i \lambda_{ij} \quad (1)$$

Here:

$$\lambda_{ij} = 2(\lambda_i^{-1} + \lambda_j^{-1})^{-1} \quad (2)$$

And:

$$\phi_i = x_i V_i / \Sigma x_j V_j \quad (3)$$

Only λ values and volumes for the pure components are needed to solve Eq. (1). Store these data, enter the mole fraction of Component 1, x_1, then press the **A** key, and λ for the mixture is calculated, displayed and printed. The thermal conductivity is given in cal/(cm)(s)(K) and Btu/(ft)(h)(°R), with the latter displayed. The x_1 value is also printed.

The programs for Eq. (1), (2) and (3) are listed in Table I, and the storage information in Table II. Calculated λ_m values are compared to experimental results for the system of methanol and water at 0°C as reported by Rastorguev and Ganier [6] in Table III.

Rather than mole fraction, the weight fraction, x_w, of components is required for the Jordan correlation [2]:

$$\frac{\lambda_m}{\lambda_1 x_{w_1} \lambda_2 x_{w_2}} = \{\exp[13.80|\lambda_2 - \lambda_1| - 0.5(13.50)(\lambda_2 + \lambda_1)]\}^{(x_{w_1} x_{w_2})} \quad (4)$$

Because mole fractions are usually more readily available than weight fractions, the program for Eq. (4) includes the conversion of x to x_w. To run this program, enter the mole fraction of Component **1**, x_1, and press **B′**. Values of the weight fractions are calculated and stored, then λ_m is calculated, displayed and printed.

If one has x_w values, they should be stored at Location **20** (x_{w_1}) and **21** (x_{w_2}), and the **B** key pressed. As in the Li program, λ_m is calculated, displayed and printed in both metric and English units.

*For information about the author, see p. 77.

The program for Eq. (4) is given in Table I, and the storage information in Table II. Calculated and experimental results for the methanol-water mixture are compared in Table III.

To predict λ_m, Vredeveld proposed [3]:

$$\lambda_m^r = x_{w_1} \lambda_1^r + x_{w_2} \lambda_2^r \quad (5)$$

Here, $r = -2$, if the difference between λ_1 and λ_2 is not greater than 2.

As does Eq. (4), Eq. (5) requires weight fractions rather than mole fractions. If one has the weight fractions, they should be stored in locations **20** and **21.** If one can use the values determined in the previous calculation, they will already be stored in these locations. Pressing **C** calculates, displays and prints λ_m.

If the composition of the mixture is known on a mole basis, enter x_1 and press **C′.** Values for x_w and λ_m will be calculated, the latter in metric and English units.

The program for Eq. (5) is listed in Table I, the storage information in Table II, and the comparison between calculated and experimental results in Table III.

For calculating λ_m, Filippov proposed [4,5]:

$$(\lambda_m - \lambda_1)/(\lambda_2 - \lambda_1) = Cx_{w_2}^2 + x_{w_2}(1 - C) \quad (6)$$

Here, C is usually set equal to 0.72, and λ_2 must be greater than λ_1.

Again, if values for x_w have been previously calculated, press **D** and λ_m will be calculated, displayed and printed. If only mole fractions are known, enter x_1 and press **D′.** The program converts mole fractions into weight fractions, then calculates λ_m.

The program for Eq. (6) is given in Table I, the storage information in Table II, and the comparison of calculated and experimental results in Table III.

To add to the utility of the foregoing programs, the Sato [3] and Riedel [7,8] correlations for predicting λ

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Programs for calculating thermal conductivities of liquid mixtures via correlations of Li, Jordan, Vredeveld and Filippov **Table I**

Li correlation

Enter x_1

Location	Code	Key
000	76	LBL
001	11	A
002	42	STO
003	06	06
004	99	PRT
005	75	-
006	01	1
007	95	=
008	94	+/-
009	42	STO
010	07	07
011	65	×
012	43	RCL
013	17	17
014	95	=
015	42	STO
016	18	18
017	85	+
018	53	(
019	43	RCL
020	06	06
021	65	×
022	43	RCL
023	16	16
024	54	)
025	95	=
026	35	1/X
027	65	×
028	43	RCL
029	18	18
030	95	=
031	42	STO
032	18	18
033	75	-
034	01	1
035	95	=
036	94	+/-
037	42	STO
038	19	19
039	65	×
040	53	(
041	02	2
042	65	×
043	53	(
044	43	RCL
045	20	20
046	35	1/X
047	85	+
048	43	RCL
049	21	21
050	35	1/X
051	54	)
052	35	1/X
053	54	)
054	65	×
055	43	RCL
056	18	18
057	65	×
058	02	2
059	95	=
060	85	+
061	53	(
062	43	RCL
063	19	19
064	33	X^2
065	65	×
066	43	RCL
067	20	20
068	54	)
069	85	+
070	53	(
071	43	RCL
072	18	18
073	33	X^2
074	65	×
075	43	RCL
076	21	21
077	54	)
078	95	=
079	99	PRT
080	55	÷
081	43	RCL
082	33	33
083	95	=
084	99	PRT
085	91	R/S

λ_m subroutine

Location	Code	Key
086	76	LBL
087	48	EXC
088	42	STO
089	06	06
090	99	PRT
091	75	-
092	01	1
093	95	=
094	94	+/-
095	42	STO
096	07	07
097	65	×
098	43	RCL
099	10	10
100	85	+
101	42	STO
102	22	22
103	53	(
104	43	RCL
105	06	06
106	65	×
107	43	RCL
108	09	09
109	54	)
110	95	=
111	35	1/X
112	65	×
113	43	RCL
114	22	22
115	95	=
116	42	STO
117	22	22
118	75	-
119	01	1
120	95	=
121	94	+/-
122	42	STO
123	23	23
124	92	RTN

Jordan correlation

Enter x_1

Location	Code	Key
125	76	LBL
126	17	B'
127	71	SBR
128	48	EXC
129	12	B
130	76	LBL
131	12	B
132	53	(
133	53	(
134	53	(
135	43	RCL
136	21	21
137	75	-
138	43	RCL
139	20	20
140	54	)
141	50	I×I
142	65	×
143	43	RCL
144	24	24
145	54	)
146	22	INV
147	23	LNX
148	75	-
149	53	(
150	93	.
151	05	5
152	65	×
153	43	RCL
154	24	24
155	65	×
156	53	(
157	43	RCL
158	21	21
159	85	+
160	43	RCL
161	20	20
162	54	)
163	54	)
164	54	)
165	45	Y^X
166	53	(
167	43	RCL
168	22	22
169	65	×
170	43	RCL
171	23	23
172	54	)
173	65	×
174	53	(
175	43	RCL
176	20	20
177	45	Y^X
178	43	RCL
179	23	23
180	65	×
181	43	RCL
182	21	21
183	45	Y^X
184	43	RCL
185	22	22
186	54	)
187	95	=
188	99	PRT
189	55	÷
190	43	RCL
191	33	33
192	95	=
193	99	PRT
194	91	R/S

Vredeveld correlation

Enter x_1

Location	Code	Key
195	76	LBL
196	18	C'
197	71	SBR
198	48	EXC
199	13	C
200	76	LBL
201	13	C
202	53	(
203	43	RCL
204	20	20
205	33	X^2
206	35	1/X
207	65	×
208	43	RCL
209	23	23
210	54	)
211	85	+
212	53	(
213	43	RCL
214	21	21
215	33	X^2
216	35	1/X
217	65	×
218	43	RCL
219	22	22
220	54	)
221	95	=
222	34	√X
223	35	1/X
224	95	=
225	99	PRT
226	55	÷
227	43	RCL
228	33	33
229	95	=
230	99	PRT
231	91	R/S

Filippov correlation

Enter x_1

Location	Code	Key
232	76	LBL
233	19	D'
234	71	SBR
235	48	EXC
236	14	D
237	76	LBL
238	14	D
239	53	(
240	43	RCL
241	22	22
242	33	X^2
243	65	×
244	43	RCL
245	25	25
246	85	+
247	43	RCL
248	22	22
249	65	×
250	53	(
251	01	1
252	75	-
253	43	RCL
254	25	25
255	54	)
256	54	)
257	65	×
258	53	(
259	43	RCL
260	21	21
261	75	-
262	43	RCL
263	20	20
264	54	)
265	95	=
266	85	+
267	43	RCL
268	20	20
269	95	=
270	99	PRT
271	55	÷
272	43	RCL
273	33	33
274	95	=
275	99	PRT
276	91	R/S

(Continued) Table I

Sato and Riedel correlations for pure components

Enter t (°C)

Location	Code	Key
277	76	LBL
278	15	E
279	99	PRT
280	85	+
281	43	RCL
282	26	26
283	95	=
284	42	STO
285	27	27
286	55	÷
287	43	RCL
288	00	00
289	95	=
290	42	STO
291	15	15
292	43	RCL
293	27	27
294	55	÷
295	43	RCL
296	03	03
297	95	=
298	42	STO
299	28	28
300	91	R/S

Enter t_{b1} (°C)

Location	Code	Key
301	99	PRT
302	85	+
303	43	RCL
304	26	26
305	95	=
306	55	÷
307	43	RCL
308	00	00
309	95	=
310	42	STO
311	11	11
312	91	R/S

Enter t_{b2} (°C)

Location	Code	Key
313	99	PRT
314	85	+
315	43	RCL
316	26	26
317	95	=
318	55	÷
319	43	RCL
320	03	03
321	95	=
322	42	STO
323	12	12
324	71	SBR
325	38	SIN
326	42	STO
327	20	20
328	99	PRT
329	43	RCL
330	09	09
331	42	STO
332	29	29
333	43	RCL
334	15	15
335	42	STO
336	30	30
337	43	RCL
338	11	11
339	42	STO
340	31	31
341	43	RCL
342	10	10
343	42	STO
344	09	09
345	43	RCL
346	28	28
347	42	STO
348	15	15
349	43	RCL
350	12	12
351	42	STO
352	11	11
353	71	SBR
354	38	SIN
355	42	STO
356	21	21
357	99	PRT
358	43	RCL
359	29	29
360	42	STO
361	09	09
362	43	RCL
363	30	30
364	42	STO
365	15	15
366	43	RCL
367	31	31
368	42	STO
369	11	11
370	91	R/S

λ subroutine

Location	Code	Key
371	76	LBL
372	38	SIN
373	53	(
374	53	(
375	53	(
376	43	RCL
377	13	13
378	65	×
379	43	RCL
380	14	14
381	54	)
382	55	÷
383	43	RCL
384	09	09
385	34	√X
386	54	)
387	65	×
388	53	(
389	53	(
390	03	3
391	85	+
392	25	CLR
393	80	GRD
394	65	×
395	53	(
396	01	1
397	75	-
398	43	RCL
399	15	15
400	54	)
401	45	Y^x
402	53	(
403	02	2
404	55	÷
405	23	LNX
406	64	PD*
407	65	65
408	55	÷
409	53	(
410	03	3
411	85	+
412	02	2
413	00	0
414	65	×
415	53	(
416	01	1
417	75	-
418	43	RCL
419	11	11
420	54	)
421	45	Y^x
422	53	(
423	02	2
424	55	÷
425	03	3
426	54	)
427	54	)
428	54	)
429	54	)
430	92	RTN

Spencer and Danner correlation for liquid volume

Enter t(°C)

Location	Code	Key
431	76	LBL
432	10	E'
433	99	PRT
434	85	+
435	43	RCL
436	26	26
437	95	=
438	42	STO
439	27	27
440	55	÷
441	43	RCL
442	00	00
443	95	=
444	42	STO
445	15	15
446	43	RCL
447	27	27
448	55	÷
449	43	RCL
450	03	03
451	95	=
452	42	STO
453	28	28
454	71	SBR
455	39	COS
456	42	STO
457	16	16
458	99	PRT
459	43	RCL
460	00	00
461	42	STO
462	29	29
463	43	RCL
464	01	01
465	42	STO
466	30	30
467	43	RCL
468	02	02
469	42	STO
470	31	31
471	43	RCL
472	15	15
473	42	STO
474	32	32
475	43	RCL
476	03	03
477	42	STO
478	00	00
479	43	RCL
480	04	04
481	42	STO
482	01	01
483	43	RCL
484	05	05
485	42	STO
486	02	02
487	43	RCL
488	28	28
489	42	STO
490	15	15
491	71	SBR
492	39	COS
493	42	STO
494	17	17
495	99	PRT
496	43	RCL
497	29	29
498	42	STO
499	00	00
500	43	RCL
501	30	30
502	42	STO
503	01	01
504	43	RCL
505	31	31
506	42	STO
507	02	02
508	43	RCL
509	32	32
510	42	STO
511	15	15
512	91	R/S

Volume subroutine

Location	Code	Key
513	76	LBL
514	39	COS
515	53	(
516	53	(
517	43	RCL
518	08	08
519	65	×
520	43	RCL
521	00	00
522	54	)
523	55	÷
524	43	RCL
525	01	01
526	54	)
527	65	×
528	53	(
529	43	RCL
530	02	02
531	45	Y^x
532	53	(
533	01	1
534	85	+
535	53	(
536	53	(
537	01	1
538	75	-
539	43	RCL
540	15	15
541	54	)
542	45	Y^x
543	53	(
544	02	2
545	55	÷
546	07	7
547	54	)
548	54	)
549	54	)
550	95	=
551	92	RTN

Nomenclature

C	Constant of Eq. (6), usually 0.72
M	Molecular weight
P	Pressure, atm
R	Gas law constant, 82.07 (cm^3)(atm)/(g-mol)(K)
T	Temperature, K
t	Temperature, °C
V	Volume, cm^3/g-mol
x	Mole fraction of component in liquid mixture
x_w	Weight fraction of component in liquid mixture
Z_{RA}	Modified critical compressibility factor for Rackett relationship
λ	Thermal conductivity, cal/(cm)(s)(K) or Btu/(ft)(h)(°R)
ϕ	Volume fraction, Eq. (3)

Subscripts

b	Normal boiling point	r	Reduced
c	Critical	s	Saturated
L	Liquid		

values for pure liquids have also been programmed:

$$\lambda_{Lb} = (2.64 \times 10^{-3})/M^{1/2} \quad (7)$$

$$\lambda_L = \left(\frac{2.64 \times 10^{-3}}{M^{1/2}}\right)\left[\frac{3 + 20(1 - T_r)^{2/3}}{3 + 20(1 - T_{rb})^{2/3}}\right] \quad (8)$$

Storage information for thermal conductivity and volume correlations — Table II

00	T_{c1}	19	ϕ_1*
01	P_{c1}	20	λ_1†
02	Z_{RA1}	21	λ_2†
03	T_{c2}	22	x_{w1}*
04	P_{c2}	23	x_{w2}*
05	Z_{RA2}	24	13.8 Constant of Eq. (4)
06	x	25	0.72 Constant of Eq. (6)
07	x_2*	26	273.16K
08	82.07, R	27	T*
09	M_1	28	For storing physical property data of Component 1, when λ and V values of Component 2 are calculated
10	M_2	29	(as above)
11	T_{rb1}	30	(as above)
12	T_{rb2}*	31	(as above)
13	2.64 Constants of Eq. (7)	32	(as above)
14	0.001 Constants of Eq. (7)	33	0.004134 Factor for converting λ values from cal/(cm)(s)(K) to Btu/(ft)(h)(°R)
15	T_{r1}*		
16	V_1†		
17	V_2†		
18	ϕ_2*		

*Calculated and stored by program

†May be calculated by program or supplied by user

Comparison of calculated and experimental values for the methanol-water system at 0°C — Table III

	λ_m, Btu/(ft)(h)(°R)				
Mol fraction water, x_1	Eq. (1)	Eq. (4)	Eq. (5)	Eq. (6)	Ref. 6
0.20	0.134	0.137	0.128	0.162	0.134
0.40	0.153	0.159	0.138	0.206	0.154
0.60	0.184	0.190	0.155	0.252	0.188
0.80	0.235	0.240	0.191	0.295	0.239

Physical properties used in calculations

	Water	Methanol
λ, Btu/(h)(ft)(°R)	0.327	0.121
V, cm^3/g-mol	18.0	37.8
Mol wt	18.015	32.042

Data sources: Ref. 1 and 9

To run the program, enter t (°C) and press **E.** Next, enter t_{b_1} and press **R/S,** then enter t_{b_2} and press **R/S.** Both λ_1 and λ_2 are calculated, stored and printed. After λ_1 is calculated, the constants for Component 2 (mol wt, T_c and T_b) are moved to replace the constants of Component 1 (which, however, are saved). After λ_2 is calculated, the constants of Component 1 are restored to their original positions.

The program and the subroutine for it are presented in Table I.

Volumes of pure components for Eq. (1) can be calculated via the Spencer-Danner modification of the Rackett equation [9]:

$$V_s = (RT_c/P_c)Z_{RA}^{[1+(1-T_r)^{2/7}]} \quad (9)$$

Although Eq. (9) provides saturated volumes, pressure differences are not likely to alter volumes much.

Enter t (°C) and press **E′,** and the volumes for two components will be calculated, stored and printed. As in the previous case, the constants for the two components are shifted as necessary, and then restored to their original locations.

Programs for λ_{L_b}, λ_L and V_s are included in Table I, and the storage information in Table II. By these programs, thermal conductivities of two-component mixtures can be calculated from a minimum amount of pure-component data—i.e., T_c, P_c, T_b and mol. wt. Of course, if thermal conductivity data for the components are available, they should be used in preference to the calculated values, and stored as indicated in Table II.

The programs and storage require both channels of two magnetic cards. Partitioning is 539.39.

For HP-67/97 Users

The listing for the HP program is contained in Table IV, with user instructions in Table V. The printout for the example can be seen in Table VI.

Program listing for HP version **Table IV**

Step	Key	Code
001	*LBLb	21 16 12
002	STO3	35 03
003	R↓	-31
004	STO4	35 04
005	R/S	51
006	STO5	35 05
007	R↓	-31
008	STO6	35 06
009	÷	-24
010	STOB	35 12
011	RCL2	36 02
012	STOI	35 46
013	RCL5	36 05
014	RCL6	36 06
015	÷	-24
016	STOC	35 13
017	GSB1	23 01
018	STO9	35 09
019	RCL4	36 04
020	RCL3	36 03
021	÷	-24
022	STOB	35 12
023	RCL1	36 01
024	STOI	35 46
025	RCL5	36 05
026	RCL3	36 03
027	÷	-24
028	STOC	35 13
029	GSB1	23 01
030	STO8	35 08
031	PRTX	-14
032	RCL9	36 09
033	PRTX	-14
034	SPC	16-11
035	R/S	51
036	*LBLc	21 16 13
037	STO3	35 03
038	1	01
039	RCL3	36 03
040	-	-45
041	STO4	35 04
042	RCL2	36 02
043	×	-35
044	ENT↑	-21
045	ENT↑	-21

Step	Key	Code
046	RCL3	36 03
047	RCL1	36 01
048	×	-35
049	+	-55
050	STOD	35 14
051	÷	-24
052	STO6	35 06
053	1	01
054	RCL6	36 06
055	-	-45
056	STO5	35 05
057	R/S	51
058	*LBLd	21 16 14
059	STO5	35 05
060	1	01
061	RCL5	36 05
062	-	-45
063	STO6	35 06
064	RCL2	36 02
065	÷	-24
066	ENT↑	-21
067	ENT↑	-21
068	RCL5	36 05
069	RCL1	36 01
070	÷	-24
071	+	-55
072	STOD	35 14
073	÷	-24
074	STO4	35 04
075	1	01
076	RCL4	36 04
077	-	-45
078	STO3	35 03
079	R/S	51
080	*LBLA	21 11
081	STO0	35 00
082	R↓	-31
083	STO7	35 07
084	RCL3	36 03
085	×	-35
086	STOI	35 46
087	RCL4	36 04
088	RCL0	36 00
089	×	-35
090	+	-55

Step	Key	Code
091	STOD	35 14
092	1	01
093	RCLI	36 46
094	RCLD	36 14
095	÷	-24
096	STOA	35 11
097	-	-45
098	STOB	35 12
099	2	02
100	RCL8	36 08
101	1/X	52
102	RCL9	36 09
103	1/X	52
104	+	-55
105	÷	-24
106	2	02
107	×	-35
108	RCLA	36 11
109	×	-35
110	RCLB	36 12
111	×	-35
112	RCLA	36 11
113	X²	53
114	RCL8	36 08
115	×	-35
116	+	-55
117	RCLB	36 12
118	X²	53
119	RCL9	36 09
120	×	-35
121	+	-55
122	GSB2	23 02
123	RCL8	36 08
124	RCL5	36 05
125	Y^X	31
126	RCL9	36 09
127	RCL6	36 06
128	Y^X	31
129	×	-35
130	RCL9	36 09
131	RCL8	36 08
132	-	-45
133	ABS	16 31
134	e^X	33
135	RCL9	36 09

Step	Key	Code
136	RCL8	36 08
137	+	-55
138	2	02
139	÷	-24
140	-	-45
141	RCL5	36 05
142	RCL6	36 06
143	×	-35
144	Y^X	31
145	×	-35
146	GSB2	23 02
147	RCL5	36 05
148	RCL8	36 08
149	X²	53
150	÷	-24
151	RCL6	36 06
152	RCL9	36 09
153	X²	53
154	÷	-24
155	+	-55
156	√X	54
157	1/X	52
158	GSB2	23 02
159	RCL8	36 08
160	RCL9	36 09
161	X≤Y?	16-35
162	R/S	51
163	.	-62
164	7	07
165	2	02
166	RCL5	36 05
167	X²	53
168	RCL5	36 05
169	-	-45
170	×	-35
171	RCL5	36 05
172	+	-55
173	RCL8	36 08
174	RCL9	36 09
175	-	-45
176	×	-35
177	RCL9	36 09
178	+	-55
179	GTO2	22 02
180	*LBL1	21 01

Step	Key	Code
181	.	-62
182	0	00
183	0	00
184	2	02
185	6	06
186	4	04
187	RCLI	36 46
188	√X	54
189	÷	-24
190	RCLE	36 15
191	÷	-24
192	1	01
193	RCLC	36 13
194	GSB3	23 03
195	×	-35
196	STOD	35 14
197	1	01
198	RCLB	36 12
199	GSB3	23 03
200	RCLD	36 14
201	X⇄Y	-41
202	÷	-24
203	RTN	24
204	*LBL3	21 03
205	-	-45
206	2	02
207	ENT↑	-21
208	3	03
209	÷	-24
210	Y^X	31
211	2	02
212	9	09
213	×	-35
214	3	03
215	+	-55
216	RTN	24
217	*LBL2	21 02
218	PRTX	-14
219	RCLE	36 15
220	÷	-24
221	PRTX	-14
222	SPC	16-11
223	RTN	24
224	R/S	51

User instructions for HP version **Table V**

Enter the following data:

Constant, 0.004134	STO **E**
Molecular weight of first component	STO **1**
Molecular weight of second component	STO **2**
Thermal conductivity, Btu/(ft)(h)(°R)	
First component	STO **8**
Second component	STO **9**

(If thermal conductivities are not available, proceed as follows and program will calculate the values using Eq. (7) and (8)):

Boiling point, K, first component	ENTER ↑
Critical temp., K, first component	key **b**
Boiling point, K, second component	ENTER ↑
Critical temp., K, second component	ENTER ↑
Test temperature, K	key **R/S**

(Continued) Table V

(Program will print the two calculated values.)

Mol fraction of first component	key **c**

(If mol fraction is not available, enter weight fraction of first component and key **d.**)

Mol volume, cm^3/g-mol, first component	ENTER ↑
Mol volume, cm^3/g-mol, second component	key **A**

Output will be the thermal conductivity of the mixture, first in Btu/(ft)(h)(°R), and then in cal/(cm)(s)(K), calculated by Eq. (1), (4), (5), and (6).

Note: Eq. (6) is only applicable if the thermal conductivity of the first component is smaller than that of the second. The program will not give the result from Eq. (6) when this condition does not hold.

Example for HP version **Table VI**

x_1 = 0.20	0.133910	***
	32.392343	***
	0.136341	***
	33.101377	***
	0.127998	***
	30.962365	***
x_1 = 0.40	0.153314	***
	37.086031	***
	0.151220	***
	33.416282	***
	0.138370	***
	33.471113	***
x_1 = 0.60	0.193611	***
	44.463070	***
	0.190911	***
	46.189742	***
	0.155540	***
	37.626064	***
x_1 = 0.80	0.234639	***
	56.772763	***
	0.241641	***
	58.707183	***
	0.190703	***
	46.130974	***

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Predict equation-of-state variables

Calculate pressure or temperature (having one or the other and volume) and resulting isothermal enthalpy change and fugacities for pure substances by means of TI-59 programs.

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☐ Programs for the Peng-Robinson [1] and Benedict-Webb-Rubin [2] equations of state presented in Part 7 of this series (Feb. 25, 1980) permit the determination of volume and compressibility factor when pressure and temperature are known, then the calculation of fugacity, isothermal enthalpy change and second and third virial coefficients for pure substances.

Given in this article are programs for these two equations that solve for pressure when volume and temperature are known and for temperature when volume and pressure are known. With the results, other programs then calculate fugacity, fugacity/pressure ratio and isothermal enthalpy change.

Peng-Robinson correlation

The Peng-Robinson equation is:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)} \qquad (1)$$

The constants a and b are generalized as follows:

$$a(T) = a(T_c) \times \alpha(T_r\omega) \qquad (2)$$

$$b(T) = b(T_c) \qquad (3)$$

Here,

$$a(T_c) = 0.45724(R^2T_c^2/P_c) \qquad (4)$$

$$b(T_c) = 0.07780(RT_c/P_c) \qquad (5)$$

$$\alpha^{1/2} = 1 + \kappa(1 - T_r^{1/2}) \qquad (6)$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \qquad (7)$$

Thus, b is a function of T_c and P_c, and $a(T)$ is a function of T_c, P_c, ω and temperature.

Determine pressure

Because the Peng-Robinson equation is explicit in P, Eq. (1) is solved directly. The constants $a(T)$ and b need only be calculated by means of Eq. (2) through (7); then, with volume and temperature known, Eq. (1) is solved. All these equations have been programmed.

To calculate pressure, enter V(L/g-mol) and press the A key. Next, enter t(°C) and press **R/S,** and pressure (atm) is calculated, displayed and printed. The results are compared to data of Canjar and Manning for methane at 37.73°C and pressures up to 170.11 atm in Table V [3].

Determine temperature

This requires a trial-and-error procedure, and the Newton technique is used to converge on the correct value of temperature. The initial estimate of temperature is determined from the ideal gas law. This calculation is included in the program.

To run the program, enter V(L/g-mol) and press the **B** key. Then enter P (atm) and press **R/S.** These quantities are printed, as well as the temperature and the cal-

Originally published January 11, 1982.

Programs for Peng-Robinson equation of state **Table I**

Location	Code	Key
Calculate P		
Enter V (L/g-mol)		
000	76	LBL
001	11	A
002	99	PRT
003	42	STO
004	19	19
005	91	R/S
Enter t(°C)		
006	99	PRT
007	85	+
008	43	RCL
009	34	34
010	95	=
011	42	STO
012	01	01
013	71	SBR
014	38	SIN
015	99	PRT
016	42	STO
017	00	00
018	91	R/S
Subroutine		
019	76	LBL
020	38	SIN
021	55	÷
022	43	RCL
023	02	02
024	95	=
025	42	STO
026	13	13
027	53	(
028	43	RCL
029	09	09
030	85	+
031	53	(
032	43	RCL
033	10	10
034	65	×
035	43	RCL
036	07	07
037	54	)
038	75	-
039	53	(
040	43	RCL
041	07	07
042	33	X²
043	65	×
044	43	RCL
045	11	11
046	54	)
047	54	)
048	42	STO
049	12	12
050	53	(
051	01	1
052	85	+
053	53	(
054	43	RCL
055	12	12
056	65	×
057	53	(
058	01	1
059	75	-
060	53	(
061	43	RCL
062	13	13
063	34	√X
064	54	)
065	54	)
066	54	)
067	54	)
068	33	X²
069	42	STO
070	14	14
071	53	(
072	53	(
073	43	RCL
074	04	04
075	65	×
076	43	RCL
077	06	06
078	33	X²
079	65	×
080	43	RCL
081	02	02
082	33	X²
083	54	)
084	55	÷
085	43	RCL
086	03	03
087	54	)
088	42	STO
089	30	30
090	65	×
091	43	RCL
092	14	14
093	95	=
094	42	STO
095	17	17
096	53	(
097	53	(
098	43	RCL
099	05	05
100	65	×
101	43	RCL
102	06	06
103	65	×
104	43	RCL
105	02	02
106	54	)
107	55	÷
108	43	RCL
109	03	03
110	54	)
111	42	STO
112	18	18
113	53	(
114	43	RCL
115	06	06
116	65	×
117	43	RCL
118	01	01
119	55	÷
120	53	(
121	43	RCL
122	19	19
123	75	-
124	43	RCL
125	18	18
126	54	)
127	54	)
128	75	-
129	53	(
130	43	RCL
131	17	17
132	55	÷
133	53	(
134	53	(
135	43	RCL
136	19	19
137	65	×
138	53	(
139	43	RCL
140	19	19
141	85	+
142	43	RCL
143	18	18
144	54	)
145	54	)
146	85	+
147	53	(
148	43	RCL
149	18	18
150	65	×
151	53	(
152	43	RCL
153	19	19
154	75	-
155	43	RCL
156	18	18
157	54	)
158	54	)
159	54	)
160	42	STO
161	20	20
162	54	)
163	95	=
164	92	RTN
Calculate T		
Enter V (L/g-mol)		
165	76	LBL
166	12	B
167	99	PRT
168	42	STO
169	19	19
170	91	R/S
Enter P (atm)		
171	99	PRT
172	42	STO
173	00	00
174	65	×
175	43	RCL
176	19	19
177	55	÷
178	43	RCL
179	06	06
180	95	=
181	42	STO
182	01	01
183	71	SBR
184	38	SIN
185	76	LBL
186	30	TAN
187	42	STO
188	08	08
189	75	-
190	43	RCL
191	00	00
192	95	=
193	50	I×I
194	75	-
195	53	(
196	43	RCL
197	00	00
198	65	×
199	93	.
200	00	0
201	00	0
202	01	1
203	54	)
204	95	=
205	77	GE
206	39	COS
207	43	RCL
208	01	01
209	75	-
210	43	RCL
211	34	34
212	95	=
213	99	PRT
214	43	RCL
215	08	08
216	99	PRT
217	91	R/S
218	76	LBL
219	39	COS
220	53	(
221	43	RCL
222	06	06
223	55	÷
224	53	(
225	43	RCL
226	19	19
227	75	-
228	43	RCL
229	18	18
230	54	)
231	54	)
232	75	-
233	53	(
234	53	(
235	43	RCL
236	30	30
237	55	÷
238	43	RCL
239	20	20
240	54	)
241	65	×
242	53	(
243	43	RCL
244	12	12
245	33	X²
246	55	÷
247	43	RCL
248	02	02
249	75	-
250	53	(
251	53	(
252	43	RCL
253	12	12
254	55	÷
255	53	(
256	43	RCL
257	01	01
258	34	√X
259	65	×
260	43	RCL
261	02	02
262	34	√X
263	54	)
264	54	)
265	54	)
266	75	-
267	53	(
268	43	RCL
269	12	12
270	33	X²
271	55	÷
272	53	(
273	43	RCL
274	01	01
275	34	√X
276	65	×
277	43	RCL
278	02	02
279	34	√X
280	54	)
281	54	)
282	54	)
283	54	)
284	95	=
285	42	STO
286	29	29
287	94	+/-
288	35	1/X
289	65	×
290	53	(
291	43	RCL
292	08	08
293	75	-
294	43	RCL
295	00	00
296	54	)
297	95	=
298	85	+
299	43	RCL
300	01	01
301	95	=
302	42	STO
303	01	01
304	71	SBR
305	38	SIN
306	61	GTO
307	30	TAN
Calculate f/p and f		
308	76	LBL
309	13	C
310	71	SBR
311	49	PRD
312	43	RCL
313	37	37
314	75	-
315	01	1
316	75	-
317	53	(
318	53	(
319	43	RCL
320	37	37
321	75	-
322	43	RCL
323	16	16
324	54	)
325	23	LNX
326	54	)
327	75	-
328	53	(
329	43	RCL
330	15	15
331	55	÷
332	53	(
333	02	2
334	65	×
335	02	2
336	34	√X
337	65	×
338	43	RCL
339	16	16
340	54	)
341	65	×
342	53	(
343	53	(
344	53	(
345	43	RCL
346	37	37
347	85	+
348	43	RCL
349	27	27
350	65	×
351	43	RCL
352	16	16
353	54	)
354	55	÷

(Continued) Table I

Location	Code	Key
355	53	(
356	43	RCL
357	37	37
358	75	-
359	43	RCL
360	28	28
361	65	×
362	43	RCL
363	16	16
364	54	)
365	54	)
366	23	LNX
367	54	)
368	54	)
369	95	=
370	22	INV
371	23	LNX
372	99	PRT
373	65	×
374	43	RCL
375	00	00
376	95	=
377	99	PRT
378	91	R/S

Subroutine

Location	Code	Key
379	76	LBL
380	49	PRD
381	53	(
382	43	RCL
383	00	00
384	65	×
385	43	RCL
386	19	19
387	54	)
388	55	÷
389	53	(
390	43	RCL
391	06	06
392	65	×
393	43	RCL
394	01	01
395	54	)
396	95	=
397	42	STO
398	37	37
399	53	(
400	43	RCL
401	17	17
402	65	×
403	43	RCL
404	00	00
405	54	)
406	55	÷
407	53	(
408	43	RCL
409	06	06
410	33	X²
411	65	×
412	43	RCL
413	01	01
414	33	X²
415	54	)
416	95	=
417	42	STO
418	15	15
419	53	(
420	43	RCL
421	18	18
422	65	×
423	43	RCL
424	00	00
425	54	)
426	55	÷
427	53	(
428	43	RCL
429	06	06
430	65	×
431	43	RCL
432	01	01
433	54	)
434	95	=
435	42	STO
436	16	16
437	92	RTN

Calculate $(H-H^*)_T$

Location	Code	Key
438	76	LBL
439	14	D
440	71	SBR
441	49	PRD
442	53	(
443	43	RCL
444	06	06
445	65	×
446	43	RCL
447	01	01
448	65	×
449	53	(
450	43	RCL
451	37	37
452	75	-
453	01	1
454	54	)
455	54	)
456	85	+
457	53	(
458	53	(
459	53	(
460	43	RCL
461	12	12
462	94	+/-
463	65	×
464	43	RCL
465	30	30
466	65	×
467	43	RCL
468	13	13
469	34	ΓX
470	54	)
471	75	-
472	53	(
473	43	RCL
474	12	12
475	33	X²
476	65	×
477	43	RCL
478	30	30
479	65	×
480	43	RCL
481	13	13
482	34	ΓX
483	54	)
484	85	+
485	53	(
486	43	RCL
487	12	12
488	33	X²
489	65	×
490	43	RCL
491	30	30
492	65	×
493	43	RCL
494	13	13
495	54	)
496	54	)
497	75	-
498	43	RCL
499	17	17
500	54	)
501	55	÷
502	53	(
503	02	2
504	65	×
505	02	2
506	34	ΓX
507	65	×
508	43	RCL
509	18	18
510	54	)
511	65	×
512	53	(
513	53	(
514	43	RCL
515	37	37
516	85	+
517	43	RCL
518	27	27
519	65	×
520	43	RCL
521	16	16
522	54	)
523	55	÷
524	53	(
525	43	RCL
526	37	37
527	75	-
528	43	RCL
529	28	28
530	65	×
531	43	RCL
532	16	16
533	54	)
534	54	)
535	23	LNX
536	54	)
537	95	=
538	65	×
539	43	RCL
540	22	22
541	95	=
542	99	PRT
543	91	R/S

Storage for Peng-Robinson equation **Table II**

Location	Data	Location	Data
00	P, atm†	19	V
01	T, K†	20	$V(V+b)+b(V-b)$*
02	T_c, K	21	–
03	P_c, atm	22	24.2179, cal/(L)(atm)
04	0.45724, constant for Eq. (4)	23	–
05	0.0778, constant for Eq. (5)	24	–
06	0.08207, R, (L)(atm)/(g-mol)(K)	25	–
07	ω	26	–
08	P, atm (in Newton method)	27	2.414
09	0.37464 } Constants for Eq. (7)	28	0.414
10	1.54226 } Constants for Eq. (7)	29	(dP/dT)* (in Newton Method)
11	0.26992 } Constants for Eq. (7)	30	$\alpha(T_c)$*
12	κ*	31	–
13	T_r^*	32	–
14	α*	33	–
15	A*	34	273.16, (0°C)
16	B*	35	–
17	a*	36	–
18	b*	37	Z*

*Calculated and stored by program

†Given or calculated, depending upon program used

Programs for Benedict-Webb-Rubin equation of state **Table III**

Calculate *P*

Enter V (L/g-mol)

Location	Code	Key
000	76	LBL
001	11	A
002	99	PRT
003	42	STO
004	13	13
005	91	R/S

Enter *t*(°C)

Location	Code	Key
006	99	PRT
007	85	+
008	43	RCL
009	20	20
010	95	=
011	42	STO
012	02	02
013	65	×
014	43	RCL
015	04	04
016	55	÷
017	43	RCL
018	13	13
019	95	=
020	71	SBR
021	38	SIN
022	99	PRT
023	42	STO
024	03	03
025	91	R/S

Subroutine

Location	Code	Key
026	76	LBL
027	38	SIN
028	85	+
029	53	(
030	53	(
031	53	(
032	43	RCL
033	06	06
034	65	×
035	43	RCL
036	04	04
037	65	×
038	43	RCL
039	02	02
040	54	)
041	75	-
042	43	RCL
043	05	05
044	75	-
045	53	(
046	43	RCL
047	07	07
048	55	÷
049	43	RCL
050	02	02
051	33	X^2
052	54	)
053	54	)
054	55	÷
055	43	RCL
056	13	13
057	33	X^2
058	54	)
059	85	+
060	53	(
061	53	(
062	53	(
063	43	RCL
064	09	09
065	65	×
066	43	RCL
067	04	04
068	65	×
069	43	RCL
070	02	02
071	54	)
072	75	-
073	43	RCL
074	08	08
075	54	)
076	55	÷
077	53	(
078	43	RCL
079	13	13
080	45	Y^X
081	03	3
082	54	)
083	54	)
084	85	+
085	53	(
086	43	RCL
087	08	08
088	65	×
089	43	RCL
090	11	11
091	55	÷
092	53	(
093	43	RCL
094	13	13
095	45	Y^X
096	06	6
097	54	)
098	54	)
099	85	+
100	53	(
101	53	(
102	43	RCL
103	10	10
104	55	÷
105	53	(
106	43	RCL
107	02	02
108	33	X^2
109	65	×
110	53	(
111	43	RCL
112	13	13
113	45	Y^X
114	03	3
115	54	)
116	54	)
117	54	)
118	65	×
119	53	(
120	01	1
121	85	+
122	53	(
123	43	RCL
124	12	12
125	55	÷
126	43	RCL
127	13	13
128	33	X^2
129	54	)
130	54	)
131	65	×
132	53	(
133	53	(
134	43	RCL
135	12	12
136	94	+/-
137	55	÷
138	43	RCL
139	13	13
140	33	X^2
141	54	)
142	22	INV
143	23	LNX
144	54	)
145	95	=
146	92	RTN

Calculate *T*

Enter V (L/g-mol)

Location	Code	Key
147	76	LBL
148	12	B
149	99	PRT
150	42	STO
151	13	13
152	91	R/S

Enter *P* (atm)

Location	Code	Key
153	99	PRT
154	42	STO
155	03	03
156	65	×
157	43	RCL
158	13	13
159	55	÷
160	43	RCL
161	04	04
162	95	=
163	42	STO
164	02	02
165	65	×
166	43	RCL
167	04	04
168	55	÷
169	43	RCL
170	13	13
171	95	=
172	76	LBL
173	30	TAN
174	71	SBR
175	38	SIN
176	42	STO
177	00	00
178	75	-
179	43	RCL
180	03	03
181	95	=
182	50	I×I
183	75	-
184	53	(
185	43	RCL
186	03	03
187	65	×
188	93	.
189	00	0
190	00	0
191	01	1
192	54	)
193	95	=
194	77	GE
195	39	COS
196	43	RCL
197	02	02
198	75	-
199	43	RCL
200	20	20
201	95	=
202	99	PRT
203	43	RCL
204	00	00
205	99	PRT
206	91	R/S
207	76	LBL
208	39	COS
209	53	(
210	43	RCL
211	04	04
212	55	÷
213	43	RCL
214	13	13
215	54	)
216	85	+
217	53	(
218	53	(
219	53	(
220	43	RCL
221	06	06
222	65	×
223	43	RCL
224	04	04
225	54	)
226	85	+
227	53	(
228	53	(
229	53	(
230	02	2
231	65	×
232	43	RCL
233	07	07
234	54	)
235	55	÷
236	53	(
237	43	RCL
238	02	02
239	45	Y^X
240	03	3
241	54	)
242	54	)
243	54	)
244	54	)
245	55	÷
246	43	RCL
247	13	13
248	33	X^2
249	54	)
250	85	+
251	53	(
252	53	(
253	43	RCL
254	09	09
255	65	×
256	43	RCL
257	04	04
258	54	)
259	55	÷
260	53	(
261	43	RCL
262	13	13
263	45	Y^X
264	03	3
265	54	)
266	54	)
267	75	-
268	53	(
269	53	(
270	53	(
271	02	2
272	65	×
273	43	RCL
274	10	10
275	54	)
276	55	÷
277	53	(
278	53	(
279	43	RCL
280	02	02
281	45	Y^X
282	03	3
283	54	)
284	65	×
285	53	(
286	43	RCL
287	13	13
288	45	Y^X
289	03	3
290	54	)
291	54	)
292	54	)
293	65	×
294	53	(
295	01	1
296	85	+
297	53	(
298	43	RCL
299	12	12
300	55	÷
301	43	RCL
302	13	13
303	33	X^2
304	54	)
305	54	)
306	65	×
307	53	(
308	53	(
309	43	RCL
310	12	12
311	94	+/-
312	55	÷
313	43	RCL
314	13	13
315	33	X^2
316	54	)
317	22	INV
318	23	LNX
319	54	)
320	54	)
321	95	=
322	42	STO
323	15	15
324	94	+/-
325	35	1/X
326	65	×
327	53	(
328	43	RCL
329	00	00
330	75	-
331	43	RCL
332	03	03
333	54	)
334	95	=
335	85	+
336	43	RCL
337	02	02
338	95	=
339	42	STO
340	02	02
341	65	×
342	43	RCL
343	04	04
344	55	÷
345	43	RCL
346	13	13
347	95	=
348	61	GTO
349	30	TAN

Calculate *f/p* and *f*

Location	Code	Key
350	76	LBL
351	13	C
352	43	RCL
353	04	04
354	65	×
355	43	RCL
356	02	02

(Continued) Table III

Location	Code	Key
357	65	×
358	53	(
359	53	(
360	43	RCL
361	04	04
362	65	×
363	43	RCL
364	02	02
365	55	÷
366	43	RCL
367	13	13
368	54	)
369	23	LNX
370	54	)
371	85	+
372	02	2
373	65	×
374	53	(
375	43	RCL
376	06	06
377	65	×
378	43	RCL
379	04	04
380	65	×
381	43	RCL
382	02	02
383	75	-
384	43	RCL
385	05	05
386	75	-
387	43	RCL
388	07	07
389	55	÷
390	43	RCL
391	02	02
392	33	X^2
393	54	)
394	55	÷
395	43	RCL
396	13	13
397	85	+
398	03	3
399	65	×
400	53	(
401	43	RCL
402	09	09
403	65	×
404	43	RCL
405	04	04
406	65	×
407	43	RCL
408	02	02
409	75	-
410	43	RCL
411	08	08
412	54	)
413	55	÷
414	02	2
415	55	÷
416	43	RCL
417	13	13
418	33	X^2
419	85	+

Location	Code	Key
420	06	6
421	65	×
422	43	RCL
423	08	08
424	65	×
425	43	RCL
426	11	11
427	55	÷
428	05	5
429	55	÷
430	53	(
431	43	RCL
432	13	13
433	45	Y^X
434	05	5
435	54	)
436	85	+
437	53	(
438	43	RCL
439	10	10
440	55	÷
441	43	RCL
442	02	02
443	33	X^2
444	55	÷
445	43	RCL
446	13	13
447	33	X^2
448	54	)
449	65	×
450	53	(
451	53	(
452	01	1
453	75	-
454	53	(
455	43	RCL
456	12	12
457	94	+/-
458	55	÷
459	43	RCL
460	13	13
461	33	X^2
462	54	)
463	22	INV
464	23	LNX
465	54	)
466	55	÷
467	43	RCL
468	12	12
469	65	×
470	43	RCL
471	13	13
472	33	X^2
473	85	+
474	53	(
475	93	.
476	05	5
477	85	+
478	43	RCL
479	12	12
480	55	÷
481	43	RCL
482	13	13

Location	Code	Key
483	33	X^2
484	54	)
485	65	×
486	53	(
487	43	RCL
488	12	12
489	94	+/-
490	55	÷
491	43	RCL
492	13	13
493	33	X^2
494	54	)
495	22	INV
496	23	LNX
497	54	)
498	95	=
499	55	÷
500	43	RCL
501	02	02
502	55	÷
503	43	RCL
504	04	04
505	95	=
506	22	INV
507	23	LNX
508	42	STO
509	17	17
510	99	PRT
511	55	÷
512	43	RCL
513	03	03
514	95	=
515	99	PRT
516	91	R/S

Calculate $(H-H^*)_T$

Location	Code	Key
517	76	LBL
518	14	D
519	53	(
520	43	RCL
521	06	06
522	65	×
523	43	RCL
524	04	04
525	65	×
526	43	RCL
527	02	03
528	75	-
529	02	2
530	65	×
531	43	RCL
532	05	05
533	75	-
534	04	4
535	65	×
536	43	RCL
537	07	07
538	55	÷
539	43	RCL
540	02	02
541	33	X^2
542	54	)

Location	Code	Key
543	55	÷
544	43	RCL
545	13	13
546	85	+
547	53	(
548	02	2
549	65	×
550	43	RCL
551	09	09
552	65	×
553	43	RCL
554	04	04
555	65	×
556	43	RCL
557	02	02
558	75	-
559	03	3
560	65	×
561	43	RCL
562	08	08
563	54	)
564	55	÷
565	02	2
566	55	÷
567	43	RCL
568	13	13
569	33	X^2
570	85	+
571	06	6
572	65	×
573	43	RCL
574	08	08
575	65	×
576	43	RCL
577	11	11
578	55	÷
579	05	5
580	55	÷
581	53	(
582	43	RCL
583	13	13
584	45	Y^X

Location	Code	Key
585	05	5
586	54	)
587	85	+
588	53	(
589	43	RCL
590	10	10
591	55	÷
592	43	RCL
593	13	13
594	33	X^2
595	55	÷
596	43	RCL
597	02	02
598	33	X^2
599	54	)
600	65	×
601	53	(
602	03	3
603	65	×
604	53	(
605	53	(
606	01	1
607	75	-
608	53	(
609	53	(
610	43	RCL
611	12	12
612	55	÷
613	43	RCL
614	13	13
615	33	X^2
616	54	)
617	94	+/-
618	22	INV
619	23	LNX
620	54	)
621	54	)
622	55	÷
623	53	(
624	43	RCL
625	12	12
626	55	÷

Location	Code	Key
627	43	RCL
628	13	13
629	33	X^2
630	54	)
631	54	)
632	75	-
633	53	(
634	93	.
635	05	5
636	75	-
637	43	RCL
638	12	12
639	55	÷
640	43	RCL
641	13	13
642	33	X^2
643	54	)
644	65	×
645	53	(
646	53	(
647	43	RCL
648	12	12
649	55	÷
650	43	RCL
651	13	13
652	33	X^2
653	54	)
654	94	+/-
655	22	INV
656	23	LNX
657	54	)
658	54	)
659	54	)
660	95	=
661	65	×
662	43	RCL
663	21	21
664	95	=
665	99	PRT
666	91	R/S

culated pressure. The degree of accuracy (i.e., the absolute difference between the calculated and given pressures) can be set as desired. In the program (Table I), the difference has been set at 0.001 (given P) (Steps **200** through **202**), but can be changed. Calculated results are again compared with data in Table V.

Calculate fugacities and enthalpy change

Using the results obtained, Program **C** in Table I calculates fugacity coefficient, f/p, and fugacity, f, and Program **D** determines the isothermal enthalpy change, $(H - H^*)_T$, with pressure. These programs are based on Eq. (11) and (12) in Part 7 (pp. 98 and 99), and, with minor changes, are the same as those listed in Table I of Part 7.

After having run **LBL A** or **LBL B** of Table I, press the **C** key to have f/p and f (atm) calculated and

Nomenclature

A, B, a, b	Constants of Eq. (1)
A_o, B_o, C_o, a, b, c, α, γ	Constants of Eq. (8)
f	Fugacity, atm
H	Enthalpy (cal/g-mol)
P	Pressure, atm
R	Gas law constant, 0.0827 (L)(atm)/(g-mol)(K)
T	Temperature, K
t	Temperature, °C
V	Volume, L/g-mol
α	Defined by Eq. (6)
κ	Defined by Eq. (7)
ω	Pitzer's acentric factor

Subscripts

c	Critical
r	Reduced

Superscript

*	Refers to ideal gas state

Storage for Benedict-Webb-Rubin equation — **Table IV**

Location	Data	Location	Data
00	P, atm (in Newton method)	13	V, L/g-mol
01	–	14	–
02	T, K†	15	(dP/dT)* (in Newton method)
03	P, atm†	16	–
04	0.08207, R, (L)(atm)/(g-mol)(K)	17	f*, atm
05	A_o (Constants of Eq. (8))	18	–
06	B_o (Constants of Eq. (8))	19	–
07	C_o (Constants of Eq. (8))	20	273.16 (0°C)
08	a (Constants of Eq. (8))	21	24.2179, cal/(L)(atm)
09	b (Constants of Eq. (8))		
10	c (Constants of Eq. (8))		
11	α (Constants of Eq. (8))		
12	γ (Constants of Eq. (8))		

*Calculated and stored by program
†Given or calculated, depending upon program used

Comparison of calculated and published equation-of-state values for methane at 37.73°C — **Table V**

		P calculated† (atm)		t calculated†† (°C)		$(H-H^*)_T$ (cal/g-mol)				
P, atm	V, L/g-mol [3]	Eq. (1)	Eq. (8)	Eq. (1)	Eq. (8)	Ref. 3	Eq. (1)†	Eq. (1)††	Eq. (8)†	Eq. (8)††
1	25.46	1.000	1.001	37.67	37.54	−1.799	−4.112	−4.113	−3.375	−3.377
13.609	1.836	13.536	13.610	39.29	37.71	−45.43	−55.69	−55.52	−46.29	−46.29
40.83	0.5891	40.179	40.734	41.89	38.31	−140.9	−164.8	−163.3	−140.6	−140.3
68.046	0.3410	66.532	67.806	42.86	38.41	−239.0	−270.1	−266.9	−236.0	−235.5
170.11	0.1279	165.08	169.19	42.94	38.64	−561.7	−594.1	−586.6	−555.2	−553.7

Physical properties of methane used in calculations

		Constants of Benedict-Webb-Rubin equation			
Mol wt	16.043	A_o	1.85500	b	0.00338004
T_c, K	191.04	B_o	0.042600	c	2545
P_c, atm	46.06	C_o	22570	α	0.000124359
ω	0.008	a	0.049400	γ	0.006

†Using V and T from Ref. 3
††Using V and P from Ref. 3

printed, and the **D** key to have $(H - H^*)_T$ (cal/g-mol) calculated and printed.

Calculated isothermal enthalpy changes are compared with published data in Table V. Two such values are reported—one based on the Peng-Robinson equation when volume and temperature are known and pressure is calculated; the other also on the same equation but when volume and pressure are known and temperature is calculated. The calculated enthalpy values differ when based on different given conditions.

All the programs based on the Peng-Robinson equation are listed in Table I and the storage information in Table II. The storage is compatible with that given in Part 7. The programs require both channels of two magnetic cards. The partitioning is 639.39.

Benedict-Webb-Rubin correlation

The Benedict-Webb-Rubin equation is:

$$P = RT/V + (B_oRT - A_o - C_o/T^2)V^2 + (bRT - a)/V^3 + a\alpha/V^6 + (c/V^3T^2)[(1 + \gamma/V^2) - \exp(-\gamma/V^2)] \quad (8)$$

Eq. (8) requires eight empirical constants, and is explicit for pressure but implicit for temperature. Hence, the general procedure for the Peng-Robinson equation applies to it as well.

To calculate pressure, enter V(L/g-mol) and press the **A** key, then enter t (°C) and press **R/S.** Values for V and t are printed, and the calculated pressure is displayed and printed. Calculated results are compared with data in Table V.

To calculate temperature, enter V and press **B,** then enter P (atm) and press **R/S.** Again, the Newton technique is used to converge on the correct temperature, the initial estimate having been calculated from the ideal gas law. As before, the degree of accuracy as a function of pressure can be set as desired. The difference has again been set at 0.001 (given P) in **Steps 189–191** in Table III, but can easily be changed.

Calculated results are again compared with data in Table V.

Fugacities and enthalpy change

Using the results obtained from Program **A** or **B** (Table III) for the Benedict-Webb-Rubin equation, f/p and f can be calculated by means of program C, and $(H - H^*)_T$ via Program **D** (Table III). The latter two programs are based on Eq. (17) and (18) in Part 7 (p. 100), and are essentially the same as those in Table III of Part 7.

Having P, V and T, press **C** to calculate and print f/p and f(atm). Press **D** and $(H - H^*)_T$ (cal/g-mol) will be calculated and printed. As with the Peng-Robinson equation, the calculated isothermal enthalpy changes will differ with different starting values for V and T or V and P. With the Benedict-Webb-Rubin equation, however, the differences will be smaller than with the Peng-Robinson equation.

All the programs for the Benedict-Webb-Rubin equation are listed in Table III, and the storage information (which is compatible with that in Part 7) in Table IV. The programs require both channels of two magnetic cards, and the partitioning is 719.29.

For HP-67/97 users

The HP version closely follows the TI program. For the Peng-Robinson equation correlation, Tables VI and VII offer program listings, and Table VIII supplies the user instructions. And, for the Benedict-Webb-Rubin equation correlation, Table X supplies the program listing, and Table XI the user instructions.

Listing for HP version—program A (Peng-Robinson equation), part 1 **Table VI**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	024	STOE	35 15	047	GSB1	23 01	070	X²	53	093	RCLD	36 14
002	SF1	16 21 01	025	STOC	35 13	048	STOC	35 13	071	RCL1	36 01	094	+	-55
003	*LBLB	21 12	026	*LBL4	21 04	049	RCLE	36 15	072	÷	-24	095	CHS	-22
004	3	03	027	.	-62	050	-	-45	073	RCL7	36 07	096	1/X	52
005	7	07	028	0	00	051	ABS	16 31	074	RCL1	36 01	097	RCLC	36 13
006	3	03	029	8	08	052	1	01	075	×	-35	098	RCLE	36 15
007	.	-62	030	2	02	053	EEX	-23	076	√X	54	099	-	-45
008	1	01	031	0	00	054	CHS	-22	077	1/X	52	100	×	-35
009	6	06	032	7	07	055	4	04	078	P⇄S	16-51	101	ST+7	35-55 07
010	STOI	35 46	033	STO6	35 06	056	RCLE	36 15	079	STO0	35 00	102	RCL7	36 07
011	R↓	-31	034	RTN	24	057	×	-35	080	P⇄S	16-51	103	GTO2	22 02
012	F1?	16 23 01	035	*LBLE	21 15	058	X>Y?	16-34	081	RCLB	36 12	104	*LBL1	21 01
013	GTOE	22 15	036	STOE	35 15	059	GTOC	22 13	082	×	-35	105	RCL1	36 01
014	STO7	35 07	037	R↓	-31	060	RCLC	36 13	083	-	-45	106	÷	-24
015	R↓	-31	038	STO4	35 04	061	RCL4	36 04	084	RCLB	36 12	107	STOA	35 11
016	STO4	35 04	039	GSB4	23 04	062	RCL5	36 05	085	X²	53	108	RCL3	36 03
017	RCLI	36 46	040	RCLE	36 15	063	-	-45	086	P⇄S	16-51	109	1	01
018	RCL7	36 07	041	RCL4	36 04	064	÷	-24	087	RCL0	36 00	110	.	-62
019	+	-55	042	×	-35	065	STOD	35 14	088	P⇄S	16-51	111	5	05
020	STO7	35 07	043	RCL6	36 06	066	RCL6	36 06	089	×	-35	112	4	04
021	GSB4	23 04	044	÷	-24	067	RCL9	36 09	090	-	-45	113	2	02
022	RCL7	36 07	045	STO7	35 07	068	÷	-24	091	×	-35	114	2	02
023	GSB1	23 01	046	*LBL2	21 02	069	RCLB	36 12	092	CHS	-22	115	6	06

(Continued) Table VI

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
116	×	-35	135	1	01	154	2	02	173	RCL4	36 04	192	RCL8	36 08
117	RCL3	36 03	136	RCLA	36 11	155	4	04	174	+	-55	193	-	-45
118	X²	53	137	√X	54	156	×	-35	175	RCL4	36 04	194	÷	-24
119	.	-62	138	-	-45	157	STO0	35 00	176	×	-35	195	+	-55
120	2	02	139	×	-35	158	RCL3	36 03	177	RCL4	36 04	196	RTN	24
121	9	09	140	1	01	159	×	-35	178	RCL8	36 08	197	*LBLC	21 13
122	6	06	141	+	-55	160	STO5	35 05	179	-	-45	198	RCLE	36 15
123	5	05	142	X²	53	161	RCL6	36 06	180	RCL8	36 08	199	PRTX	-14
124	2	02	143	STO9	35 09	162	RCL1	36 01	181	×	-35	200	RCL7	36 07
125	×	-35	144	RCL6	36 06	163	×	-35	182	+	-55	201	RCLI	36 46
126	-	-45	145	RCL1	36 01	164	RCL2	36 02	183	STO9	35 09	202	-	-45
127	.	-62	146	×	-35	165	÷	-24	184	1/X	52	203	PRTX	-14
128	3	03	147	X²	53	166	.	-62	185	RCL5	36 05	204	SPC	16-11
129	7	07	148	RCL2	36 02	167	0	00	186	×	-35	205	CF1	16 22 01
130	4	04	149	÷	-24	168	7	07	187	CHS	-22	206	R/S	51
131	6	06	150	.	-62	169	7	07	188	RCL5	36 05			
132	4	04	151	4	04	170	6	06	189	RCL7	36 07			
133	+	-55	152	5	05	171	×	-35	190	×	-35			
134	STOB	35 12	153	7	07	172	STO8	35 08	191	RCL4	36 04			

Listing for HP version—program A (Peng-Robinson equation), part 2 **Table VII**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	027	STO3	35 03	053	-	-45	079	STOD	35 14	105	2	02
002	RCLE	36 15	028	RCL1	36 01	054	÷	-24	080	RCLB	36 12	106	√X	54
003	RCL4	36 04	029	1	01	055	LN	32	081	X²	53	107	÷	-24
004	×	-35	030	-	-45	056	STOC	35 13	082	RCL0	36 00	108	RCL8	36 08
005	RCL6	36 06	031	RCL1	36 01	057	RCL2	36 02	083	×	-35	109	÷	-24
006	÷	-24	032	RCL3	36 03	058	2	02	084	RCLA	36 11	110	RCLC	36 13
007	RCL7	36 07	033	-	-45	059	÷	-24	085	×	-35	111	×	-35
008	÷	-24	034	LN	32	060	2	02	086	RCLB	36 12	112	RCLD	36 14
009	STO1	35 01	035	-	-45	061	√X	54	087	RCL0	36 00	113	+	-55
010	RCL5	36 05	036	STO9	35 09	062	÷	-24	088	×	-35	114	2	02
011	RCLE	36 15	037	RCL1	36 01	063	RCL3	36 03	089	RCLA	36 11	115	4	04
012	×	-35	038	2	02	064	÷	-24	090	√X	54	116	.	-62
013	RCL6	36 06	039	.	-62	065	RCLC	36 13	091	×	-35	117	2	02
014	X²	53	040	4	04	066	×	-35	092	-	-45	118	1	01
015	÷	-24	041	1	01	067	CHS	-22	093	RCLB	36 12	119	7	07
016	RCL7	36 07	042	4	04	068	RCL9	36 09	094	X²	53	120	9	09
017	X²	53	043	RCL3	36 03	069	+	-55	095	RCL0	36 00	121	×	-35
018	÷	-24	044	×	-35	070	e^x	33	096	×	-35	122	RCL9	36 09
019	STO2	35 02	045	+	-55	071	STO9	35 09	097	RCLA	36 11	123	PRTX	-14
020	RCL8	36 08	046	RCL1	36 01	072	RCL6	36 06	098	√X	54	124	RCLE	36 15
021	RCLE	36 15	047	.	-62	073	RCL7	36 07	099	×	-35	125	×	-35
022	×	-35	048	4	04	074	×	-35	100	-	-45	126	PRTX	-14
023	RCL6	36 06	049	1	01	075	RCL1	36 01	101	RCL5	36 05	127	R↓	-31
024	÷	-24	050	4	04	076	1	01	102	-	-45	128	PRTX	-14
025	RCL7	36 07	051	RCL3	36 03	077	-	-45	103	2	02	129	SPC	16-11
026	÷	-24	052	×	-35	078	×	-35	104	÷	-24	130	R/S	51

User instructions for HP version—program A (Peng-Robinson equation) — Table VIII

1. Enter program card for part 1	
2. Enter critical temperature, K, T_c	**STO 1**
3. Enter critical pressure, atm, P_c	**STO 2**
4. Enter acentric factor, ω	**STO 3**
5. Enter volume V, L/g-mol	**ENTER ↑**
6. Enter pressure P, atm	**Key A**
or	
Temperature t, °C	**Key B**
Output will be:	
Pressure P, atm	
Temperature t, °C	
7. Enter program card for part 2	**Key A**
Output will be:	
Fugacity coefficient, f/p	
Fugacity f, atm	
Enthalpy change $(H - H^*)_T$, cal/g-mol.	

Note: To do another calculation, start from beginning.

Listing for HP version—program B (Benedict-Webb-Rubin equation), part 1 — Table IX

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	045	RCLI	36 46	089	RCL8	36 08	133	÷	-24	177	÷	-24
002	SF1	16 21 01	046	-	-45	090	RCLA	36 11	134	LN	32	178	5	05
003	*LBLB	21 12	047	3	03	091	X²	53	135	RCL9	36 09	179	÷	-24
004	STOA	35 11	048	×	-35	092	÷	-24	136	×	-35	180	6	06
005	R↓	-31	049	ST+9	35-55 09	093	STOE	35 15	137	RCL0	36 00	181	×	-35
006	F1?	16 23 01	050	RCL9	36 09	094	+	-55	138	×	-35	182	+	-55
007	GTO4	22 04	051	GTO5	22 05	095	RCLE	36 15	139	RCL2	36 02	183	STOD	35 14
008	STOB	35 12	052	*LBL3	21 03	096	CHS	-22	140	RCL0	36 00	184	1	01
009	RCLA	36 11	053	RCL2	36 02	097	e^x	33	141	×	-35	185	RCLE	36 15
010	×	-35	054	RCL0	36 00	098	STOE	35 15	142	RCL9	36 09	186	-	-45
011	RCL0	36 00	055	×	-35	099	×	-35	143	×	-35	187	RCL8	36 08
012	÷	-24	056	RCL9	36 09	100	STOD	35 14	144	RCL1	36 01	188	RCLA	36 11
013	STO9	35 09	057	×	-35	101	R↓	-31	145	-	-45	189	X²	53
014	GTO5	22 05	058	RCL1	36 01	102	RCL6	36 06	146	RCL3	36 03	190	÷	-24
015	*LBL4	21 04	059	-	-45	103	RCLA	36 11	147	RCL9	36 09	191	STOC	35 13
016	P⇄S	16-51	060	RCL3	36 03	104	3	03	148	X²	53	192	÷	-24
017	RCL0	36 00	061	RCL9	36 09	105	Y^x	31	149	÷	-24	193	RCLC	36 13
018	P⇄S	16-51	062	X²	53	106	÷	-24	150	-	-45	194	.	-62
019	+	-55	063	÷	-24	107	RCL9	36 09	151	2	02	195	5	05
020	STO9	35 09	064	-	-45	108	X²	53	152	×	-35	196	+	-55
021	*LBL5	21 05	065	RCLA	36 11	109	÷	-24	153	RCLA	36 11	197	RCLE	36 15
022	RCLA	36 11	066	X²	53	110	RCLD	36 14	154	÷	-24	198	×	-35
023	÷	-24	067	÷	-24	111	×	-35	155	+	-55	199	+	-55
024	RCL0	36 00	068	RCL5	36 05	112	+	-55	156	RCL5	36 05	200	RCL6	36 06
025	×	-35	069	RCL0	36 00	113	RTN	24	157	RCL0	36 00	201	RCL9	36 09
026	STOC	35 13	070	×	-35	114	*LBL6	21 06	158	×	-35	202	X²	53
027	GSB3	23 03	071	RCL9	36 09	115	RCLC	36 13	159	RCL9	36 09	203	÷	-24
028	F1?	16 23 01	072	×	-35	116	+	-55	160	×	-35	204	RCLA	36 11
029	GTO6	22 06	073	RCL4	36 04	117	STOB	35 12	161	RCL4	36 04	205	X²	53
030	RCLC	36 13	074	-	-45	118	*LBL7	21 07	162	-	-45	206	÷	-24
031	+	-55	075	RCLA	36 11	119	RCLB	36 12	163	3	03	207	×	-35
032	STOI	35 46	076	3	03	120	PRTX	-14	164	×	-35	208	RCLD	36 14
033	RCLB	36 12	077	Y^x	31	121	RCL9	36 09	165	2	02	209	+	-55
034	-	-45	078	÷	-24	122	P⇄S	16-51	166	÷	-24	210	RCL9	36 09
035	ABS	16 31	079	+	-55	123	RCL0	36 00	167	RCLA	36 11	211	÷	-24
036	1	01	080	RCL4	36 04	124	P⇄S	16-51	168	X²	53	212	RCL0	36 00
037	EEX	-23	081	RCL7	36 07	125	-	-45	169	÷	-24	213	÷	-24
038	CHS	-22	082	×	-35	126	PRTX	-14	170	+	-55	214	e^x	33
039	3	03	083	RCLA	36 11	127	SPC	16-11	171	RCL4	36 04	215	PRTX	-14
040	RCLB	36 12	084	6	06	128	CF1	16 22 01	172	RCL7	36 07	216	RCLB	36 12
041	×	-35	085	Y^x	31	129	RCL0	36 00	173	×	-35	217	÷	-24
042	X>Y?	16-34	086	÷	-24	130	RCL9	36 09	174	RCLA	36 11	218	PRTX	-14
043	GTO7	22 07	087	+	-55	131	×	-35	175	5	05	219	SPC	16-11
044	RCLB	36 12	088	1	01	132	RCLA	36 11	176	Y^x	31	220	R/S	51

Listing for HP version—program B (Benedict-Webb-Rubin equation), part 2 **Table X**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	018	RCLA	36 11	035	5	05	052	RCLE	36 15	069	÷	-24
002	RCL2	36 02	019	÷	-24	036	×	-35	053	-	-45	070	RCL9	36 09
003	RCL0	36 00	020	RCL5	36 05	037	+	-55	054	3	03	071	X²	53
004	×	-35	021	2	02	038	RCL7	36 07	055	×	-35	072	÷	-24
005	RCL9	36 09	022	×	-35	039	RCL4	36 04	056	RCLC	36 13	073	RCLI	36 46
006	×	-35	023	RCL0	36 00	040	×	-35	057	÷	-24	074	+	-55
007	RCL1	36 01	024	×	-35	041	RCLA	36 11	058	.	-62	075	2	02
008	2	02	025	RCL9	36 09	042	5	05	059	5	05	076	4	04
009	×	-35	026	×	-35	043	Yˣ	31	060	RCLC	36 13	077	.	-62
010	-	-45	027	RCL4	36 04	044	÷	-24	061	-	-45	078	2	02
011	RCL3	36 03	028	3	03	045	6	06	062	RCLE	36 15	079	1	01
012	4	04	029	×	-35	046	×	-35	063	×	-35	080	7	07
013	×	-35	030	-	-45	047	5	05	064	-	-45	081	9	09
014	RCL9	36 09	031	RCLA	36 11	048	÷	-24	065	RCL6	36 06	082	×	-35
015	X²	53	032	X²	53	049	+	-55	066	×	-35	083	PRTX	-14
016	÷	-24	033	÷	-24	050	STOI	35 46	067	RCLA	36 11	084	SPC	16-11
017	-	-45	034	.	-62	051	1	01	068	X²	53	085	R/S	51

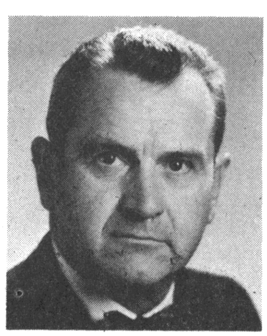
User instructions for HP version—program B (Benedict-Webb-Rubin equation) **Table XI**

Enter program card for part 1	
Enter gas constant, °R (0.08207)	**STO 0**
Enter equation constants:	
A_0	**STO 1**
B_0	**STO 2**
C_0	**STO 3**
a	**STO 4**
b	**STO 5**
c	**STO 6**
α	**STO 7**
γ	**STO 8**
Switch storage registers	Key **f P⇄S**
Enter temperature constant, 273.16	**STO 0** (secondary register)
	Key **f P⇄2**
Enter temperature *t*, °C	**ENTER ↑**
Volume *V*, L/g-mol.	Key **A**
or	
Enter pressure *P*, atm	**ENTER ↑**
Volume *V*, L/g-mol.	Key **B**
Output will be:	
Pressure, atm	
Temperature, °C	
Fugacity *f*, atm	
Fugacity coefficient *f*/*p*	
Enter program card for part 2 (side 1 only)	Key **A**
Output will be:	
Enthalpy change, $(H - H^*)$, cal/g-mol.	

Note: To do another calculation, start from beginning.

References

1. Peng, D. Y., and Robinson, D. R., *Ind. Eng. Chem. Fund.*, Vol. 15, 1976, p. 59.
2. Benedict, M., Webb, G. B., and Rubin, L. C., *J. Chem. Phys.*, Vol. 8, 1940, p. 334.
3. Canjar, L. N., and Manning, F. S., "Thermodynamic Properties and Reduced Correlations for Gases," Gulf Pub. Co., Houston, Tex., 1967.



The author

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Holder of B.S., M.S. and Ph.D. degrees in chemical engineering from the University of Pittsburgh, he is a member of AIChE and ACS, a registered engineer in the State of Nebraska, and author or coauthor of 60 articles published in technical and scientific magazines.

Predict gas-phase diffusion coefficients

Relationships are presented for determining diffusion coefficients for mixtures of nonpolar gases and mixtures containing polar gases. These are programmed for the TI-59 calculator.

*James H. Weber, University of Nebraska**

☐ Diffusion coefficients for non-polar gas systems may be found via correlations of Chapman and Cowling [*3*], Wilke and Lee [*9*], and Fuller, Schettler and Giddings [*4*]. Those for mixtures containing polar gases may be determined by means of the modifications to the Chapman-Cowling correlation proposed by Brokaw [*1*].

Note that gas-phase diffusion coefficients are independent of composition.

Chapman-Cowling relationship

Coefficients for mixtures of nonpolar gases may be calculated by means of the basic relationship of Chapman and Cowling:

$$D_{12} = (0.001858T^{3/2})\left\{\frac{[(M_1 + M_2)/(M_1M_2)]^{1/2}}{P\sigma_{12}^2\Omega_D}\right\} \quad (1)$$

According to Neufeld, Janzen and Aziz [*5*]:

$$\Omega_D = \frac{A}{T^{*B}} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)} \quad (2)$$

$$T^* = kT/\varepsilon_{12} \quad (3)$$

$$\varepsilon_{12} = (\varepsilon_1\varepsilon_2)^{1/2} \quad (4)$$

$$\sigma_{12} = (\sigma_1 + \sigma_2)/2 \quad (5)$$

Eq. (1) through (5) have been programmed. The pure component properties M, ε and σ are stored. To calculate and display D_{12}, enter P (atm) and press **A,** then enter t (°C) and press **R/S.**

The program is listed in Table I and the storage information in Table II. For the ethane and *n*-hexane system at atmospheric pressure, calculated results are compared with experimental data of Carmichael, Sage and Lacey [*2*] in Table VI.

***For information about the author, see p. 77.**

Wilke-Lee modification

Wilke and Lee modified Eq. (1) by substituting for 0.001858 the term:

$$0.00217 - 0.00050[(M_1 + M_2)/(M_1M_2)]^{1/2}$$

To determine D_{12} using this modification, enter P (atm) and press **B,** then enter t (°C) and press **R/S.** The diffusion coefficient (cm²/s) is calculated, displayed and printed, and P and t also are printed. The program is listed in Table I and the storage information in Table II. Calculated and experimental results for the ethane and *n*-hexane system are compared in Table VI.

Fuller-Schettler-Giddings correlation

Diffusion coefficients may also be calculated by means of the Fuller-Schettler-Giddings relationship:

$$D_{12} = (0.001\,T^{1.75})\left\{\frac{[(M_1 + M_2)/(M_1M_2)]^{1/2}}{P[(\Sigma V)_1^{1/3} + (\Sigma V)_2^{1/3}]^2}\right\} \quad (6)$$

The terms V_1 and V_2 are "atomic diffusion volumes." These may be estimated from data given in Table III.

To calculate D_{12} values via Eq. (6), estimate values for $(\Sigma V)_1$ and $(\Sigma V)_2$ and store them in Locations **35** and **36.** To calculate, display and print D_{12} (cm²/s), enter P (atm) and press **C,** then enter t (°C) and press **R/S.**

The program is listed in Table I and the storage information in Table II. Results for the ethane and *n*-hexane system are compared in Table VI.

Note that in the three relationships discussed, the diffusion coefficient is inversely proportional to the absolute pressure. This proportionality is valid for a number of systems at low or moderate pressure. At high pressure, more-complex methods must be used.

Originally published May 3, 1982.

Programs for calculating diffusion coefficients by Chapman-Cowling, Wilke-Lee, and Fuller-Schettler-Giddings correlations and σ and ε/k by Tee-Gotoh-Stewart correlations **Table I**

Location	Code	Key
Chapman-Cowling correlation		
Enter *P* (atm)		
000	76	LBL
001	11	A
Enter *t*(°C)		
002	71	SBR
003	48	EXC
004	65	×
005	43	RCL
006	23	23
007	65	×
008	71	SBR
009	38	SIN
010	95	=
011	55	÷
012	71	SBR
013	47	CMS
014	95	=
015	99	PRT
016	91	R/S
Subroutine SIN		
017	76	LBL
018	38	SIN
019	53	(
020	53	(
021	43	RCL
022	02	02
023	85	+
024	43	RCL
025	06	06
026	54	)
027	55	÷
028	53	(
029	43	RCL
030	02	02
031	65	×
032	43	RCL
033	06	06
034	54	)
035	54	)
036	34	√X
037	92	RTN
Subroutine COS		
038	76	LBL
039	39	COS
040	53	(
041	43	RCL
042	09	09
043	55	÷
044	53	(
045	43	RCL
046	30	30
047	65	×
048	43	RCL
049	31	31
050	54	)
051	34	√X
052	54	)
053	42	STO
054	14	14
055	92	RTN
Subroutine TAN		
056	76	LBL
057	30	TAN
058	53	(
059	53	(
060	43	RCL
061	15	15
062	55	÷
063	53	(
064	43	RCL
065	14	14
066	45	Y^x
067	43	RCL
068	16	16
069	54	)
070	54	)
071	85	+
072	53	(
073	43	RCL
074	17	17
075	55	÷
076	53	(
077	53	(
078	43	RCL
079	18	18
080	65	×
081	43	RCL
082	14	14
083	54	)
084	22	INV
085	23	LNX
086	54	)
087	54	)
088	85	+
089	53	(
090	43	RCL
091	19	19
092	55	÷
093	53	(
094	53	(
095	43	RCL
096	20	20
097	65	×
098	43	RCL
099	14	14
100	54	)
101	22	INV
102	23	LNX
103	54	)
104	54	)
105	85	+
106	53	(
107	43	RCL
108	21	21
109	55	÷
110	53	(
111	53	(
112	43	RCL
113	22	22
114	65	×
115	43	RCL
116	14	14
117	54	)
118	22	INV
119	23	LNX
120	54	)
121	54	)
122	54	)
123	42	STO
124	12	12
125	92	RTN
Subroutine EXC		
126	76	LBL
127	48	EXC
128	99	PRT
129	42	STO
130	08	08
131	91	R/S
132	99	PRT
133	85	+
134	43	RCL
135	34	34
136	95	=
137	53	(
138	42	STO
139	09	09
140	45	Y^x
141	53	(
142	01	1
143	93	.
144	05	5
145	54	)
146	54	)
147	92	RTN
Subroutine CMS		
148	76	LBL
149	47	CMS
150	53	(
151	43	RCL
152	08	08
153	65	×
154	53	(
155	53	(
156	43	RCL
157	32	32
158	85	+
159	43	RCL
160	33	33
161	54	)
162	55	÷
163	02	2
164	54	)
165	33	X^2
166	65	×
167	71	SBR
168	39	COS
169	71	SBR
170	30	TAN
171	54	)
172	92	RTN
Wilke-Lee correlation		
Enter *P* (atm)		
173	76	LBL
174	12	B
Enter *t*(°C)		
175	71	SBR
176	48	EXC
177	42	STO
178	13	13
179	53	(
180	53	(
181	43	RCL
182	24	24
183	75	-
184	53	(
185	43	RCL
186	25	25
187	65	×
188	71	SBR
189	38	SIN
190	54	)
191	54	)
192	65	×
193	43	RCL
194	13	13
195	65	×
196	71	SBR
197	38	SIN
198	54	)
199	55	÷
200	71	SBR
201	47	CMS
202	95	=
203	99	PRT
204	91	R/S
Fuller-Shettler-Giddings correlation		
Enter *P* (atm)		
205	76	LBL
206	13	C
207	99	PRT
208	42	STO
209	08	08
210	91	R/S
Enter *t*(°C)		
211	99	PRT
212	85	+
213	43	RCL
214	34	34
215	95	=
216	45	Y^x
217	53	(
218	01	1
219	93	.
220	07	7
221	05	5
222	54	)
223	65	×
224	93	.
225	00	0
226	00	0
227	01	1
228	65	×
229	71	SBR
230	38	SIN
231	95	=
232	55	÷
233	53	(
234	43	RCL
235	08	08
236	65	×
237	53	(
238	53	(
239	43	RCL
240	35	35
241	45	Y^x
242	53	(
243	01	1
244	55	÷
245	03	3
246	54	)
247	54	)
248	85	+
249	53	(
250	43	RCL
251	36	36
252	45	Y^x
253	53	(
254	01	1
255	55	÷
256	03	3
257	54	)
258	54	)
259	54	)
260	33	X^2
261	54	)
262	95	=
263	99	PRT
264	91	R/S
Tee-Gotoh-Stewart correlations		
265	76	LBL
266	14	D
267	53	(
268	53	(
269	43	RCL
270	26	26
271	75	-
272	53	(
273	43	RCL
274	27	27
275	65	×
276	43	RCL
277	03	03
278	54	)
279	54	)
280	65	×
281	53	(
282	43	RCL
283	00	00
284	55	÷
285	43	RCL
286	01	01
287	54	)
288	45	Y^x
289	53	(
290	01	1
291	55	÷
292	03	3
293	54	)
294	54	)
295	42	STO
296	32	32
297	99	PRT
298	53	(
299	53	(
300	43	RCL
301	26	26
302	75	-
303	53	(
304	43	RCL
305	27	27
306	65	×
307	43	RCL
308	07	07
309	54	)
310	54	)
311	65	×
312	53	(
313	43	RCL
314	04	04
315	55	÷
316	43	RCL
317	05	05
318	54	)
319	45	Y^x
320	53	(
321	01	1
322	55	÷
323	03	3
324	54	)
325	54	)
326	42	STO
327	33	33
328	99	PRT
329	53	(
330	53	(
331	43	RCL
332	28	28
333	85	+

(Continued) Table I

Location	Code	Key	Location	Code	Key	Location	Code	Key
334	43	RCL	345	30	30	356	07	07
335	29	29	346	99	PRT	357	54	)
336	65	×	347	53	(	358	65	×
337	43	RCL	348	53	(	359	43	RCL
338	03	03	349	43	RCL	360	04	04
339	54	)	350	28	28	361	54	)
340	65	×	351	85	+	362	99	PRT
341	43	RCL	352	43	RCL	363	42	STO
342	00	00	353	29	29	364	31	31
343	54	)	354	65	×	365	91	R/S
344	42	STO	355	43	RCL			

Nomenclature

A, B, C, D, E, F, G, H	Constants of Eq. (2)
D	Diffusion coefficient, cm^2/s
M	Molecular weight
P	Pressure, atm
T	Temperature, K
T^*	Defined by Eq. (3)
t	Temperature, °C
V	Volume, cm^3/g-mol
δ	Polar parameter, defined by Eq. (10)
ε	Energy parameter
μ_p	Dipole moment, debyes
σ	Length parameter, Å
Ω_D	Collision integral for diffusion

Subscripts

1,2	Components 1 and 2
b	Normal boiling point

Storage information for correlations for diffusion coefficients in non-polar systems — Table II

00	T_{c1}	19	1.03587, E — Constants of Eq. (2) (cont'd)
01	P_{c1}	20	1.52996, F — Constants of Eq. (2) (cont'd)
02	M_1	21	1.76474, G — Constants of Eq. (2) (cont'd)
03	ω_1	22	3.89411, H — Constants of Eq. (2) (cont'd)
04	T_{c2}	23	0.001858 Constant of Eq. (1)
05	P_{c2}	24	0.00217 — Constants for Wilke-Lee correlation
06	M_2	25	0.0005 — Constants for Wilke-Lee correlation
07	ω_2	26	2.3551 — Constants of Eq. (7)
08	P	27	0.087 — Constants of Eq. (7)
09	T^*	28	0.7915 — Constants of Eq. (8)
10	Not used	29	0.1693 — Constants of Eq. (8)
11	Not used	30	$(\epsilon/k)_1$††
12	Ω_D* Defined by Eq. (2)	31	$(\epsilon/k)_2$††
13	Not used	32	σ_1††
14	(T^*)†	33	σ_2††
15	1.06036, A — Constants of Eq. (2)	34	273.16 (0° C)
16	0.1561, B — Constants of Eq. (2)	35	ΣV_A
17	0.193, C — Constants of Eq. (2)	36	ΣV_B
18	0.47635, D — Constants of Eq. (2)		

† Values calculated and stored per pressures

†† Values calculated and stored by program, or supplied by user

Atomic diffusion volumes for Fuller-Schettler-Giddings correlation — Table III

Atomic and structural diffusion volume increments, v

C	16.5	Cl†	19.5
H	1.98	S†	17.0
O	5.48	Aromatic ring	−20.2
N†	5.69	Heterocyclic ring	20.2

Diffusion volumes for simple molecules, Σv

H_2	7.07	CO	18.9
D_2	6.70	CO_2	26.9
He	2.88	N_2O	35.9
N_2	17.9	NH_3	14.9
O_2	16.6	H_2O	12.7
Air	20.1	CCl_2F_2†	114.8
Ar	16.1	SF_6†	69.7
Kr	22.8	Cl_2†	37.7
Xe†	37.9	Br_2†	67.2
		SO_2†	41.1

† Based on a few data points.

Values for σ and ε may be estimated by the relationships proposed by Tee, Gotoh and Stewart [8]:

$$\sigma(P_c/T_c)^{1/3} = 2.3551 - 0.087\omega \qquad (7)$$

and

$$\varepsilon/kT_c = 0.7915 + 0.1693\omega \qquad (8)$$

Assuming the fundamental data T_c, P_c and ω are stored in the proper locations, σ_1, σ_2, $(\varepsilon/k)_1$ and $(\varepsilon/k)_2$ may be calculated by means of Eq. (7) and (8) by pressing **D.** The values of the constants are calculated, stored in the proper locations, and printed. The calculation of D_{12} can then proceed as has been described.

The programs for Eq. (7) and (8) are listed in Table I, and the storage information in Table II. The programs and storage require both channels of two magnetic cards. Partitioning is normal.

Brokaw modification for polar gases

For mixtures containing polar gases, Brokaw suggested that diffusion coefficients be calculated by means

Programs for calculating diffusion coefficients for mixtures containing polar substances via Brokaw correlations, δ, σ and ϵ/k by Brokaw method, and boiling points and volumes by Spencer-Danner method **Table IV**

Location	Code	Key
Calculate D_{12} for mixtures with polar substances via Brokaw correlations		
Enter P (atm)		
000	76	LBL
001	11	A
002	99	PRT
003	42	STO
004	08	08
005	91	R/S
Enter t(°C)		
006	99	PRT
007	85	+
008	43	RCL
009	34	34
010	95	=
011	53	(
012	42	STO
013	09	09
014	45	Y^X
015	53	(
016	01	1
017	93	.
018	05	5
019	54	)
020	54	)
021	65	×
022	43	RCL
023	23	23
024	65	×
025	53	(
026	53	(
027	43	RCL
028	02	02
029	85	+
030	43	RCL
031	06	06
032	54	)
033	55	÷
034	53	(
035	43	RCL
036	02	02
037	65	×
038	43	RCL
039	06	06
040	54	)
041	54	)
042	34	√X
043	95	=
044	55	÷
045	53	(
046	43	RCL
047	08	08
048	65	×
049	53	(
050	43	RCL
051	32	32
052	65	×
053	43	RCL
054	33	33
055	54	)
056	65	×
057	53	(
058	43	RCL
059	09	09
060	55	÷
061	53	(
062	43	RCL
063	30	30
064	65	×
065	43	RCL
066	31	31
067	54	)
068	34	√X
069	54	)
070	42	STO
071	14	14
072	53	(
073	53	(
074	53	(
075	43	RCL
076	15	15
077	55	÷
078	53	(
079	43	RCL
080	14	14
081	45	Y^X
082	43	RCL
083	16	16
084	54	)
085	54	)
086	85	+
087	53	(
088	43	RCL
089	17	17
090	55	÷
091	53	(
092	53	(
093	43	RCL
094	18	18
095	65	×
096	43	RCL
097	14	14
098	54	)
099	22	INV
100	23	LNX
101	54	)
102	54	)
103	85	+
104	53	(
105	43	RCL
106	19	19
107	55	÷
108	53	(
109	53	(
110	43	RCL
111	20	20
112	65	×
113	43	RCL
114	14	14
115	54	)
116	22	INV
117	23	LNX
118	54	)
119	54	)
120	85	+
121	53	(
122	43	RCL
123	21	21
124	55	÷
125	53	(
126	53	(
127	43	RCL
128	22	22
129	65	×
130	43	RCL
131	14	14
132	54	)
133	22	INV
134	23	LNX
135	54	)
136	54	)
137	54	)
138	42	STO
139	12	12
140	85	+
141	53	(
142	53	(
143	93	.
144	01	1
145	09	9
146	65	×
147	53	(
148	43	RCL
149	37	37
150	33	X²
151	54	)
152	54	)
153	55	÷
154	43	RCL
155	14	14
156	54	)
157	54	)
158	54	)
159	95	=
160	99	PRT
161	91	R/S
Calculate δ for pure components and mixtures, and σ and ϵ/k for pure components by Brokaw method		
162	76	LBL
163	12	B
164	53	(
165	53	(
166	43	RCL
167	49	49
168	65	×
169	43	RCL
170	38	38
171	33	X²
172	54	)
173	55	÷
174	53	(
175	43	RCL
176	44	44
177	65	×
178	43	RCL
179	40	40
180	54	)
181	54	)
182	42	STO
183	35	35
184	99	PRT
185	53	(
186	53	(
187	43	RCL
188	49	49
189	65	×
190	43	RCL
191	39	39
192	33	X²
193	54	)
194	55	÷
195	53	(
196	43	RCL
197	45	45
198	65	×
199	43	RCL
200	41	41
201	54	)
202	54	)
203	99	PRT
204	42	STO
205	36	36
206	65	×
207	43	RCL
208	35	35
209	95	=
210	34	√X
211	99	PRT
212	42	STO
213	37	37
214	53	(
215	53	(
216	43	RCL
217	11	11
218	65	×
219	43	RCL
220	44	44
221	54	)
222	55	÷
223	53	(
224	01	1
225	85	+
226	43	RCL
227	43	43
228	65	×
229	43	RCL
230	35	35
231	33	X²
232	54	)
233	42	STO
234	46	46
235	54	)
236	45	Y^X
237	53	(
238	01	1
239	55	÷
240	03	3
241	54	)
242	95	=
243	42	STO
244	32	32
245	99	PRT
246	53	(
247	53	(
248	43	RCL
249	11	11
250	65	×
251	43	RCL
252	45	45
253	54	)
254	55	÷
255	53	(
256	01	1
257	85	+
258	43	RCL
259	43	43
260	65	×
261	43	RCL
262	36	36
263	33	X²
264	54	)
265	42	STO
266	47	47
267	54	)
268	45	Y^X
269	53	(
270	01	1
271	55	÷
272	03	3
273	54	)
274	95	=
275	42	STO
276	33	33
277	99	PRT
278	53	(
279	43	RCL
280	42	42
281	65	×
282	43	RCL
283	40	40
284	65	×
285	43	RCL
286	46	46
287	54	)
288	99	PRT
289	42	STO
290	30	30
291	53	(
292	43	RCL
293	42	42
294	65	×
295	43	RCL
296	41	41
297	65	×
298	43	RCL
299	47	47
300	54	)
301	99	PRT
302	42	STO
303	31	31
304	91	R/S
Calculate normal boiling point (K) and liquid volumes via Spencer-Danner method		
Enter t_{b1}(°C)		
305	76	LBL
306	18	C'
307	99	PRT
308	85	+
309	43	RCL
310	34	34
311	95	=
312	42	STO
313	40	40
314	91	R/S
Enter t_{b2}(°C)		
315	99	PRT
316	85	+
317	43	RCL
318	34	34
319	95	=
320	42	STO
321	41	41
322	91	R/S
Enter t_{b1}(°C)		
323	76	LBL
324	13	C
325	99	PRT
326	85	+
327	43	RCL
328	34	34
329	95	=
330	42	STO
331	09	09
332	42	STO
333	40	40
334	71	SBR
335	60	DEG
336	42	STO
337	44	44
338	99	PRT
339	91	R/S
Enter t_{b2}(°C)		
340	99	PRT
341	85	+
342	43	RCL
343	34	34
344	95	=
345	42	STO
346	41	41
347	42	STO
348	09	09

(Continued) Table IV

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
349	43	RCL	364	00	00	379	52	52	392	60	DEG	407	50	50	422	54	)
350	00	00	365	43	RCL	380	42	STO	393	53	(	408	45	Y^X	423	45	Y^X
351	42	STO	366	05	05	381	00	00	394	53	(	409	53	(	424	53	(
352	52	52	367	42	STO	382	43	RCL	395	43	RCL	410	01	1	425	02	2
353	43	RCL	368	01	01	383	53	53	396	13	13	411	85	+	426	55	÷
354	01	01	369	43	RCL	384	42	STO	397	65	×	412	53	(	427	07	7
355	42	STO	370	51	51	385	01	01	398	43	RCL	413	01	1	428	54	)
356	53	53	371	42	STO	386	43	RCL	399	00	00	414	75	-	429	54	)
357	43	RCL	372	50	50	387	54	54	400	55	÷	415	53	(	430	54	)
358	50	50	373	71	SBR	388	42	STO	401	43	RCL	416	43	RCL	431	54	)
359	42	STO	374	60	DEG	389	50	50	402	01	01	417	09	09	432	92	RTN
360	54	54	375	42	STO	390	91	R/S	403	54	)	418	55	÷			
361	43	RCL	376	45	45				404	65	×	419	43	RCL			
362	04	04	377	99	PRT	Subroutine DEG			405	53	(	420	00	00			
363	42	STO	378	43	RCL	391	76	LBL	406	43	RCL	421	54	)			

Storage information for calculating diffusion coefficients of systems containing polar compounds **Table V**

00	T_{c_1}	23	0.001858 Constant of Eq. (1)	46	$(1{+}1.3\,\delta^2)_1$†
01	P_{c_1}	24	Not used	47	$(1{+}1.3\,\delta^2)_2$†
02	M_1	25	Not used	48	Not used
03	Not used	26	Not used	49	1940 Constant of Eq. (10)
04	T_{c_2}	27	Not used	50	Z_{RA_1}
05	P_{c_2}	28	Not used	51	Z_{RA_2}
06	M_2	29	Not used	52	Used for storing T_{c_1}, P_{c_1} and M_1
07	Not used	30	$(\epsilon/k)_1$††	53	Used for storing T_{c_1}, P_{c_1} and M_1
08	P	31	$(\epsilon/k)_2$††	54	Used for storing T_{c_1}, P_{c_1} and M_1
09	T†	32	σ_1††		
10	Not used	33	σ_2††		
11	1.585 Constant of Eq. (12)	34	273.16 (0° C)		
12	Ω_D† Defined by Eq. (9)	35	δ_1††		
13	82.07 (R)	36	δ_2††		
14	(T^*)†	37	δ_{12}††		
15	1.0636, A — Constants of Eq. 2	38	μ_{p_1}		
16	0.1561, B — Constants of Eq. 2	39	μ_{p_2}		
17	0.193, C — Constants of Eq. 2	40	T_{b_1}††		
18	0.47635, D — Constants of Eq. 2	41	T_{b_2}††		
19	1.03587, E — Constants of Eq. 2	42	1.18		
20	1.52996, F — Constants of Eq. 2	43	1.3		
21	1.76474, G — Constants of Eq. 2	44	V_1††		
22	3.89411, H — Constants of Eq. 2	45	V_2††		

† Calculated and stored by program
†† Calculated and stored by program, or supplied by user
Note: This storage has been made compatible with that in Table II

of the basic relationship Eq. (1) with the following modifications:

$$\Omega_D = \Omega_D\,[\text{Eq. (2)}] + [0.19(\delta_{12})^2/T^*] \qquad (9)$$

with

$$\delta = [(1940\mu_p^2)/V_b T_b] \qquad (10)$$

$$\varepsilon/k = 1.18(1 + 1.3\delta^2)T_b \qquad (11)$$

$$\sigma = [1.585 V_b/(1 + 1.3\delta^2)]^{1/3} \qquad (12)$$

$$\delta_{12} = (\delta_1\delta_2)^{1/2} \qquad (13)$$

$$\varepsilon_{12}/k = [(\varepsilon_1/k)(\varepsilon_2/k)]^{1/2} \qquad (14)$$

$$\sigma_{12} = (\sigma_1\sigma_2)^{1/2} \qquad (15)$$

Eq. (1), with the modifications required by Eq. (9) through (15), has been programmed. Diffusion coefficients may be calculated by entering P (atm) and pressing **A**, then entering t (°C) and pressing **R/S.** Assuming that the necessary properties are known and stored in their proper locations, the diffusion coefficient will be calculated, displayed and printed.

The program is listed in Table IV and the storage information in Table V. For an ammonia and diethyl ether system, calculated results are compared in Table VI with experimental data of B. N. and I. B. Srivastava [7]. As for nonpolar substances, the diffusion coefficient is inversely proportional to the absolute pressure at low or moderate pressure.

Calculating required properties

With the exception of the dipole moment, μ_p, the values of the properties required to determine diffusion

Comparison of calculated and experimental values for diffusion coefficients **Table VI**

System: ethane and *n*-hexane* (P = 1 atm)

t, °C	Chapman-Cowling	Wilke-Lee	Fuller-Schettler-Gidding	Carmichael-Sage-Lacey
	D_{12}, cm²/s			
21.1	0.0485	0.0539	0.0597	0.0391
37.8	0.0541	0.0602	0.0658	0.0498
54.4	0.0601	0.0667	0.0721	0.0597
71.1	0.0663	0.0737	0.0786	0.0690
87.8	0.0728	0.0809	0.0854	0.0781
104.4	0.0795	0.0884	0.0924	0.0869

Note: For this system, the diffusion coefficient at a specific temperature is inversely proportional to the absolute pressure, over a modest pressure range

*Values of σ and ϵ/k calculated via Eq. (7) and (8)

System: ammonia and diethyl ether† (P = 1 atm)

t, °C	Eq. (1), Brokaw modification	Srivastava
15.14	0.0881	0.0999
64.34	0.1214	0.137

†Values of σ, ϵ/k, and δ calculated by Eq. (10)-(12)

Physical properties used in calculations

	Ethane	*n*-Hexane	Ammonia	Diethyl ether
M	30.070	86.178	17.031	74.123
T_b, (K)	184.5	341.9	239.1	307.7
T_c, (K)	305.4	507.4	405.6	466.7
P_c, atm	48.2	29.3	111.3	35.9
μ_p, debyes	–	–	1.5	1.3
Z_{RA}			0.24658	0.26444
ω	0.098	0.296	0.250	0.281
ΣV	44.88	126.72	–	–

Data sources: Reid, R. C., Prausnitz, J. M., and Sherwood, T. K., "The Properties of Gases and Liquids," 3rd ed., McGraw-Hill, Inc., New York, 1977, and Spencer, C. F., and Adler, S. B., *J. Chem. Eng. Data*, Vol. 23, 1978. p. 82.

coefficients may be calculated from fundamental data, T_c, P_c, t_b and Z_{RA}. Programs have been included to calculate δ_1, δ_2, δ_{12}, $(\varepsilon/k)_1$, $(\varepsilon/k)_2$, σ_1, σ_2, V_{b_1} and V_{b_2}.

First, a program calculates T_b values from t_b values. Enter t_{b_1} and press **C**′, and T_{b_1} is calculated, stored and displayed. Next, enter t_{b_2} and press **R/S**, and T_{b_2} is calculated, stored and displayed.

Volumes can be calculated by the Spencer and Danner modification [6] of the Rackett correlation:

$$V_b = (RT_c/P_c)Z_{RA}^{[1+(1-T_r)^{2/7}]} \tag{16}$$

Enter t_{b_1} and press **C**, and V_{b_1} is calculated, stored, displayed and printed. Next, enter t_{b_2} and press **R/S**, and V_{b_2} is calculated, stored, displayed and printed.

The required data are now available to calculate values for δ, (ε/k) and σ. Press **B** to calculate, print and store (in the proper locations for the calculation of D_{12}) values for: δ_1 and δ_2—via Eq. (10); δ_{12}—via Eq. (13); $(\varepsilon/k)_1$ and $(\varepsilon/k)_2$—via Eq. (11); σ_1 and σ_2—via Eq. (12). Programs for calculating these properties are included in Table IV, and the storage information in Table V. As far as possible, the storage information in Table V and II has been made compatible.

All the programs and storage for calculating coefficients for systems containing polar compounds can be placed on two magnetic cards. Partitioning is normal.

For HP-67/97 users

Because the HP program consists of two parts, it is not possible to calculate diffusion coefficients at different temperatures and pressures simply by entering a different temperature and pressure. After the diffusion coefficient of a gaseous mixture has been calculated at a certain temperature and pressure, program A must be entered again into the calculator to calculate the diffusion coefficient at another temperature and pressure.

The results produced by the HP programs will agree within 10% with those of the TI program. As with the TI program, the HP results tend to be higher than the experimental data of Carmichael, Sage and Lacey at lower temperatures, and tend to be lower than the experimental data at higher temperatures.

Tables VII and VIII contain HP program listings, and Table IX offers user instructions.

Listing for HP version—program A **Table VII**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	015	RCLI	36 46	029	P⇄S	16-51	043	STOD	35 14	057	÷	-24
002	SF1	16 21 01	016	×	-35	030	GSB4	23 04	044	P⇄S	16-51	058	Y^x	31
003	*LBLB	21 12	017	√X	54	031	GTO6	22 06	045	GSB7	23 07	059	1	01
004	RCLA	36 11	018	STOI	35 46	032	*LBL1	21 01	046	GTO6	22 06	060	+	-55
005	+	-55	019	GSB3	23 03	033	GSB5	23 05	047	*LBL2	21 02	061	Y^x	31
006	STOA	35 11	020	STOC	35 13	034	STOC	35 13	048	RCL5	36 05	062	RCLD	36 14
007	R↓	-31	021	P⇄S	16-51	035	P⇄S	16-51	049	1	01	063	×	-35
008	STOB	35 12	022	GSB3	23 03	036	GSB5	23 05	050	RCL4	36 04	064	RCL0	36 00
009	F1?	16 23 01	023	RCLC	36 13	037	RCLC	36 13	051	RCL0	36 00	065	×	-35
010	GTO1	22 01	024	×	-35	038	+	-55	052	÷	-24	066	RCL1	36 01
011	GSB2	23 02	025	√X	54	039	2	02	053	–	-45	067	÷	-24
012	STOI	35 46	026	STOC	35 13	040	÷	-24	054	2	02	068	STO7	35 07
013	P⇄S	16-51	027	GSB4	23 04	041	STOC	35 13	055	ENT↑	-21	069	1/X	52
014	GSB2	23 02	028	STOD	35 14	042	GSB7	23 07	056	7	07	070	1	01

(Continued) Table VII

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
071	9	09	102	÷	-24	133	RCL8	36 08	164	RCLD	36 14	195	6	06
072	4	04	103	Y^x	31	134	X^2	53	165	x	-35	196	3	03
073	0	00	104	RTN	24	135	x	-35	166	$\sqrt{X}$	54	197	5	05
074	x	-35	105	*LBL5	21 05	136	1	01	167	STOD	35 14	198	x	-35
075	RCL6	36 06	106	2	02	137	+	-55	168	RCLA	36 11	199	e^x	33
076	X^2	53	107	.	-62	138	1	01	169	RCLD	36 14	200	÷	-24
077	x	-35	108	3	03	139	.	-62	170	÷	-24	201	+	-55
078	RCL4	36 04	109	5	05	140	1	01	171	STOE	35 15	202	1	01
079	÷	-24	110	5	05	141	8	08	172	1	01	203	.	-62
080	STO8	35 08	111	1	01	142	x	-35	173	.	-62	204	0	00
081	RTN	24	112	RCL3	36 03	143	RCL4	36 04	174	0	00	205	3	03
082	*LBL3	21 03	113	.	-62	144	x	-35	175	6	06	206	5	05
083	1	01	114	6	06	145	RTN	24	176	0	00	207	8	08
084	.	-62	115	8	08	146	*LBL7	21 07	177	3	03	208	7	07
085	5	05	116	7	07	147	RCL3	36 03	178	6	06	209	RCLE	36 15
086	8	08	117	x	-35	148	.	-62	179	RCLE	36 15	210	1	01
087	5	05	118	-	-45	149	1	01	180	.	-62	211	.	-62
088	RCL7	36 07	119	RCL1	36 01	150	6	06	181	1	01	212	5	05
089	x	-35	120	RCL0	36 00	151	9	09	182	5	05	213	2	02
090	1	01	121	÷	-24	152	3	03	183	6	06	214	9	09
091	.	-62	122	1	01	153	x	-35	184	1	01	215	9	09
092	3	03	123	ENT↑	-21	154	.	-62	185	Y^x	31	216	6	06
093	RCL8	36 08	124	3	03	155	7	07	186	÷	-24	217	x	-35
094	X^2	53	125	÷	-24	156	9	09	187	.	-62	218	e^x	33
095	x	-35	126	Y^x	31	157	1	01	188	1	01	219	÷	-24
096	1	01	127	÷	-24	158	5	05	189	9	09	220	+	-55
097	+	-55	128	RTN	24	159	+	-55	190	3	03	221	CF1	16 22 01
098	÷	-24	129	*LBL4	21 04	160	RCL0	36 00	191	RCLE	36 15	222	R/S	51
099	1	01	130	1	01	161	x	-35	192	.	-62			
100	ENT↑	-21	131	.	-62	162	RTN	24	193	4	04			
101	3	03	132	3	03	163	*LBL6	21 06	194	7	07			

Listing for HP version—program B **Table VIII**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	027	.	-62	053	÷	-24	079	1	01	105	x	-35
002	SF1	16 21 01	028	1	01	054	RCLA	36 11	080	7	07	106	STO9	35 09
003	*LBLB	21 12	029	9	09	055	3	03	081	RCLD	36 14	107	RCL7	36 07
004	1	01	030	x	-35	056	ENT↑	-21	082	.	-62	108	1	01
005	.	-62	031	RCLE	36 15	057	2	02	083	0	00	109	ENT↑	-21
006	7	07	032	÷	-24	058	÷	-24	084	0	00	110	3	03
007	6	06	033	+	-55	059	Y^x	31	085	0	00	111	÷	-24
008	4	04	034	*LBL7	21 07	060	x	-35	086	5	05	112	Y^x	31
009	7	07	035	RCLB	36 12	061	STOE	35 15	087	x	-35	113	RCL8	36 08
010	4	04	036	x	-35	062	.	-62	088	-	-45	114	1	01
011	RCLE	36 15	037	RCLC	36 13	063	0	00	089	RCLE	36 15	115	ENT↑	-21
012	3	03	038	X^2	53	064	0	00	090	x	-35	116	3	03
013	.	-62	039	x	-35	065	1	01	091	PRTX	-14	117	÷	-24
014	8	08	040	STOC	35 13	066	8	08	092	R/S	51	118	Y^x	31
015	9	09	041	RCL2	36 02	067	5	05	093	RCLD	36 14	119	+	-55
016	4	04	042	ENT↑	-21	068	8	08	094	RCLA	36 11	120	RCLB	36 12
017	1	01	043	P⇄S	16-51	069	x	-35	095	1	01	121	x	-35
018	1	01	044	RCL2	36 02	070	PRTX	-14	096	.	-62	122	X^2	53
019	x	-35	045	+	-55	071	F1?	16 23 01	097	7	07	123	RCL9	36 09
020	e^x	33	046	X⇄Y	-41	072	GTO1	22 01	098	5	05	124	X⇄Y	-41
021	÷	-24	047	RCL2	36 02	073	R/S	51	099	Y^x	31	125	÷	-24
022	+	-55	048	x	-35	074	*LBL1	21 01	100	x	-35	126	PRTX	-14
023	F1?	16 23 01	049	÷	-24	075	.	-62	101	.	-62	127	R/S	51
024	GTO7	22 07	050	$\sqrt{X}$	54	076	0	00	102	0	00			
025	RCLI	36 46	051	STOD	35 14	077	0	00	103	0	00			
026	X^2	53	052	RCLC	36 13	078	2	02	104	1	01			

User Instructions for HP version — Table IX

Steps	Keys
Enter program A	
Enter the following data:	
Temperature constant, 273.16	STO A
Gas constant, 82.07	STO D
First component of gas mixture:	
Critical temperature, T_c, K	STO 0
Critical pressure, P_c, atm	STO 1
Molecular weight	STO 2
Acentric factor, ω	STO 3
(For polar gases)	
Boiling point, T_b, K	STO 4
Compressibility factor, Z_{RA}	STO 5
Dipole moment, μ_p	STO 6
Switch data into secondary registers	P ⇌ S
Enter data for second component	
Run part 1 of program:	
Enter pressure, atm	ENTER ↑
Enter temperature, °C	
For nonpolar gases	A
For polar gases	B
When the calculator stops, enter program B.	

Run program by pressing **A** for nonpolar gases or **B** for polar gases. Output will be diffusivity coefficient, cm^2/s, first by Chapman-Cowling correlation, then by Wilke-Lee correlation.

To calculate the diffusivity coefficient via Fuller-Schettler-Giddings correlation:

Enter ΣV_1	STO 7
Enter ΣV_2	STO 8
Press	R/S

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Predict liquid-phase diffusion coefficients

Programs for the TI-59 calculator determine diffusion coefficients in dilute two-component solutions.

*James H. Weber, University of Nebraska**

☐ Diffusion coefficients in liquid phases, unlike those in vapor phases, depend on concentration. The relationships presented are only valid for dilute solutions—i.e., solute concentrations no greater than 10%. Indeed, the lower the solute concentration, the more accurate the calculated coefficient. Because of the concentration dependence, the solute and solvent must be specified. In this article, solute is called Component A, and solvent, Component B.

A number of correlations have been suggested for predicting diffusion coefficients in dilute liquid solutions. Of these, three are programmed here: the Wilke-Chang [*1*], Scheibel [*2*] and Reddy-Doraiswamy [*3*].

Wilke-Chang relationship

Wilke and Chang proposed:

$$D^o_{AB} = 7.4 \times 10^{-8}[(\phi M_B)^{1/2}T/\eta_B V_A^{0.6}] \quad (1)$$

The dimensionless quantity ϕ is the association factor of the solvent. Its value is 1—except for water, 2.6; methanol, 1.9; and ethanol, 1.5.

The program for Eq. (1) is listed in Table I. If values for the required variables have been stored in the locations designated in Table II, D^o_{AB} (in cm^2/s) will be calculated, printed and displayed by entering t (°C) and pressing the **A** key. Calculated and experimental results for cyclohexane (solute) and benzene (solvent) are compared in Table III.

Scheibel relationship

Eq. (2) and (3) represent Scheibel's correlation:

$$D^o_{AB} = KT/\eta_B V_A^{1/3} \quad (2)$$

$$K = (8.2 \times 10^{-8})[1 + (3V_B/V_A)^{2/3}] \quad (3)$$

Eq. (3) applies generally; three exceptions are: $K = 25.2 \times 10^{-8}$, when water is the solvent, and $V_A < V_B$; $K = 19.8 \times 10^{-8}$, when benzene is the solvent, and $V_A < 2V_B$; and $K = 17.5 \times 10^{-8}$ for solvents other than water and benzene, when $V_A < 2.5\ V_B$.

Pressing **B′** will calculate, display, print and store (at Location 09) $K \times 10^8$. (Note that the factor 10^{-8} is taken into account in subsequent calculations.) This value is used in the determination of D^o_{AB}, except in the three special cases just cited.

After $K \times 10^8$ has been computed and stored, D^o_{AB} is calculated, displayed and printed by entering t (°C) and pressing **B**. Programs for Eq. (2) and (3) are listed in Table I, and the storage information in Table II. Calculated and experimental results are again compared in Table III.

Reddy-Doraiswamy relationship

Reddy and Doraiswamy proposed:

$$D^o_{AB} = K'M_B^{1/2}T/\eta_B(V_A V_B)^{1/3} \quad (4)$$

Here, $K' = 10 \times 10^{-8}$ if $V_B/V_A < 1.5$; and 8.5×10^{-8} if $V_B/V_A > 1.5$.

The program for Eq. (4) includes the selection and storage of the proper value of K' (Table I and II). Therefore, to calculate, display and print D^o_{AB} (cm^2/s), enter t (°C) and press **C**.

Calculated and experimental results are again compared in Table III.

Liquid volume and viscosity

In the preceding calculation, the liquid volume at the normal boiling point of both the solute and solvent may be required, and the liquid viscosity of the solvent at temperature t is required. To facilitate the computation of D^o_{AB}, programs for calculating these two properties are included in Table I.

Programmed for liquid volumes is the modification of the Rackett equation by Danner and Spencer [*6*]:

$$V_S = (RT_c/P_c)Z_{RA}^{[1+(1-T_r)^{2/7}]} \quad (5)$$

To calculate, display, print and store V_A (cm^3/g-mol), enter t_{bA} (°C) and press **D**. To calculate, print and store V_B, enter t_{bB} (°C) and press **R/S**. To have V_B displayed, the command **RCL 03** must be inserted before **R/S** at Step 180.

If viscosity is not known, it can be estimated by Thomas's relationship [*7*]:

$$\log[8.569(\eta_L/\rho_L^{1/2})] = \theta[(1/T_r) - 1] \quad (6)$$

Listed in Table I is the program for Eq. (6) and the

*For information about the author, see p. 77.

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Programs for calculating D^o_{AB} by the Wilke-Chang, Scheibel, and Reddy-Doraiswamy correlations, and for finding liquid volume and viscosity **Table I**

Wilke-Chang correlation

Enter t(°C)

Location	Code	Key
000	76	LBL
001	11	A
002	99	PRT
003	85	+
004	43	RCL
005	08	08
006	95	=
007	42	STO
008	05	05
009	65	×
010	53	(
011	43	RCL
012	04	04
013	65	×
014	43	RCL
015	00	00
016	54	)
017	34	$\sqrt{x}$
018	65	×
019	43	RCL
020	07	07
021	65	×
022	43	RCL
023	06	06
024	95	=
025	55	÷
026	53	(
027	43	RCL
028	01	01
029	65	×
030	43	RCL
031	02	02
032	45	Y^x
033	93	.
034	06	6
035	54	)
036	95	=
037	99	PRT
038	91	R/S

Scheibel correlation

Enter t(°C)

Location	Code	Key
039	76	LBL
040	12	B
041	99	PRT
042	85	+
043	43	RCL
044	08	08
045	95	=
046	42	STO
047	05	05
048	65	×
049	43	RCL
050	09	09
051	65	×
052	43	RCL
053	06	06
054	95	=
055	55	÷
056	53	(
057	43	RCL
058	01	01
059	65	×
060	43	RCL
061	02	02
062	45	Y^x
063	53	(
064	01	1
065	55	÷
066	03	3
067	54	)
068	54	)
069	95	=
070	99	PRT
071	91	R/S

Reddy-Doraiswamy correlation

Enter t(°C)

Location	Code	Key
072	76	LBL
073	13	C
074	99	PRT
075	85	+
076	43	RCL
077	08	08
078	95	=
079	42	STO
080	05	05
081	71	SBR
082	30	TAN
083	43	RCL
084	05	05
085	65	×
086	43	RCL
087	00	00
088	34	$\sqrt{x}$
089	65	×
090	43	RCL
091	10	10
092	65	×
093	43	RCL
094	06	06
095	95	=
096	55	÷
097	53	(
098	43	RCL
099	01	01
100	65	×
101	53	(
102	43	RCL
103	02	02
104	65	×
105	43	RCL
106	03	03
107	54	)
108	45	Y^x
109	53	(
110	01	1
111	55	÷
112	03	3
113	54	)
114	95	=
115	99	PRT
116	91	R/S

Spencer-Danner correlation

Enter t_{bA}(°C)

Location	Code	Key
117	76	LBL
118	14	D
119	99	PRT
120	85	+
121	43	RCL
122	08	08
123	95	=
124	42	STO
125	20	20
126	71	SBR
127	38	SIN
128	99	PRT
129	42	STO
130	02	02
131	91	R/S

Enter t_{bB}(°C)

Location	Code	Key
132	99	PRT
133	85	+
134	43	RCL
135	08	08
136	95	=
137	42	STO
138	20	20
139	43	RCL
140	11	11
141	42	STO
142	17	17
143	43	RCL
144	12	12
145	42	STO
146	18	18
147	43	RCL
148	13	13
149	42	STO
150	19	19
151	43	RCL
152	14	14
153	42	STO
154	11	11
155	43	RCL
156	15	15
157	42	STO
158	12	12
159	43	RCL
160	16	16
161	42	STO
162	13	13
163	71	SBR
164	38	SIN
165	42	STO
166	03	03
167	99	PRT
168	43	RCL
169	17	17
170	42	STO
171	11	11
172	43	RCL
173	18	18
174	42	STO
175	12	12
176	43	RCL
177	19	19
178	42	STO
179	13	13
180	91	R/S

Subroutine SIN

Location	Code	Key
181	76	LBL
182	38	SIN
183	53	(
184	53	(
185	43	RCL
186	21	21
187	65	×
188	43	RCL
189	11	11
190	55	÷
191	43	RCL
192	12	12
193	54	)
194	65	×
195	53	(
196	43	RCL
197	13	13
198	45	Y^x
199	53	(
200	01	1
201	85	+
202	53	(
203	01	1
204	75	−
205	53	(
206	43	RCL
207	20	20
208	55	÷
209	43	RCL
210	11	11
211	54	)
212	54	)
213	45	Y^x
214	53	(
215	02	2
216	55	÷
217	07	7
218	54	)
219	54	)
220	54	)
221	54	)
222	92	RTN

Thomas correlation

Enter t(°C)

Location	Code	Key
223	76	LBL
224	15	E
225	99	PRT
226	85	+
227	43	RCL
228	08	08
229	95	=
230	55	÷
231	43	RCL
232	14	14
233	95	=
234	42	STO
235	22	22
236	53	(
237	53	(
238	43	RCL
239	21	21
240	65	×
241	43	RCL
242	14	14
243	55	÷
244	43	RCL
245	15	15
246	54	)
247	65	×
248	53	(
249	43	RCL
250	16	16
251	45	Y^x
252	53	(
253	01	1
254	85	+
255	53	(
256	01	1
257	75	−
258	43	RCL
259	22	22
260	54	)
261	45	Y^x
262	53	(
263	02	2
264	55	÷
265	07	7
266	54	)
267	54	)
268	54	)
269	54	)
270	55	÷
271	43	RCL
272	00	00
273	95	=
274	35	1/X
275	34	$\sqrt{x}$
276	42	STO
277	23	23
278	53	(
279	53	(
280	43	RCL
281	22	22
282	35	1/X
283	75	−
284	01	1
285	54	)
286	65	×
287	43	RCL
288	24	24
289	54	)
290	22	INV
291	28	LOG
292	65	×
293	53	(
294	43	RCL
295	23	23
296	55	÷
297	43	RCL
298	25	25
299	54	)
300	95	=
301	42	STO
302	01	01
303	99	PRT
304	91	R/S

***K* via Eq. (3)**

Location	Code	Key
305	76	LBL
306	17	B'
307	53	(
308	53	(
309	53	(
310	03	3
311	65	×
312	43	RCL
313	03	03
314	55	÷
315	43	RCL
316	02	02
317	54	)
318	45	Y^x
319	53	(
320	02	2
321	55	÷
322	03	3
323	54	)
324	54	)
325	85	+
326	01	1
327	54	)
328	65	×
329	08	8
330	93	.
331	02	2
332	95	=
333	42	STO
334	09	09
335	99	PRT
336	91	R/S

Subroutine TAN

Location	Code	Key
337	76	LBL
338	30	TAN
339	53	(
340	43	RCL
341	03	03
342	55	÷
343	43	RCL
344	02	02
345	54	)
346	75	−
347	43	RCL
348	26	26
349	95	=
350	77	GE
351	39	COS
352	01	1
353	00	0
354	42	STO
355	10	10
356	00	0
357	77	GE
358	31	LRN
359	08	8
360	93	.
361	05	5
362	42	STO
363	10	10
364	92	RTN

Storage information for Table I programs **Table II**

00	M_B	10	K'^*, Reddy-Doraiswamy constant	20	T_b^*, Boiling point, K
01	$\mu_B^\dagger$	11	T_{cA}	21	82.07 = R
02	$V_A^\dagger$	12	P_{cA}	22	T_{rb}^*
03	$V_B^\dagger$	13	$(Z_{RA})_A$	23	$\rho_L^{1/2*}$
04	ϕ	14	T_{cB}	24	θ, Thomas constant
05	T^*	15	P_{cB}	25	8.569, Eq. (6) constant
06	0.00000001	16	$(Z_{RA})_B$	26	1.499 Ratio of V_B/V_A—used in determination of K' value in solution of Eq. (4)
07	7.4, Eq. (1) constant	17	Used for storing properties of Component A during calculations of V_B		
08	273.16 (0°C)	18			
09	$K^\dagger$, Scheibel constant	19			

*Calculated and stored by program
†Calculated and stored by program or supplied by user

Comparison of calculated and experimental coefficient values for cyclohexane-benzene system **Table III**

D^o_{AB} values are in 10^{-5} cm²/s

t, °C	Wilke-Chang	Scheibel	Reddy-Doraiswamy	Sanni, et al.
25	1.84*	1.89*	1.93*	2.09
	2.82†	2.90†	2.97†	
40	2.39*	2.46*	2.51*	2.65
	3.41†	3.51†	3.59†	
60	3.13*	3.22*	3.29*	3.45
	4.30†	4.43†	4.52†	

*Experimental values of viscosity for benzene, used in calculating coefficient
†Viscosity values calculated via Eq. (6), used in calculating coefficient

Physical properties used in calculations

	Cyclohexane	Benzene
M	84.162	78.114
T_c, K	553.4	562.1
P_c, atm	40.2	48.3
T_b, K	353.9	353.3
Z_{RA}	0.27286	0.26967
θ		0.634
η, cP		0.609 (25°C)
		0.492 (40°C)
		0.400 (60°C)

Data sources: Reid, R. C., Prausnitz, J.M., and Sherwood, T. K., "Properties of Gases and Liquids," 3rd ed., McGraw-Hill Inc., 1977; Spencer, C. F., and Adler, S. B., *J. Chem. Eng. Data*, Vol. 23, 1978, p. 82; API Project 44, Carnegie Press, Pittsburgh, 1953.

Atomic and group contributions to calculation of θ, Eq. (6) [7] **Table IV**

Carbon	−0.462	Sulfur	0.043
Hydrogen	0.249	Double bond	0.478
Oxygen	0.054	C_6H_5–	0.385
Chlorine	0.340	CO (ketones, esters)	0.105
Bromine	0.326	CN (cyanides)	0.381
Iodine	0.335		

Nomenclature

- D^o_{AB} Diffusion coefficient, cm²/s
- K Constant, Eq. (3)
- K' Constant, Eq. (4)
- M Molecular weight
- R Gas law constant, 82.07 (atm)(cm³)/(g-mol)(K)
- T Absolute temperature, K
- V Molal volume at normal boiling point, cm³/g-mol
- Z_{RA} Rackett compressibility factor
- θ Thomas viscosity constant, Eq. (6) and Table IV
- η Viscosity, cP
- ρ Density, g/cm³
- ϕ Association factor, Eq. (1)

Superscripts

- o Infinite dilution

Subscripts

- A Solute
- B Solvent
- c Critical
- L Liquid
- r Reduced

Spencer-Danner correlation for calculating density. Also, θ, which must be stored in Location 24, can be determined from data given in Table IV. Viscosity can now be displayed, printed and stored by entering t (°C) and pressing E.

Partitioning is normal (459.59). The programs and storage information require both tracks of one card and one track of a second.

Note that, in all the correlations given, the diffusion coefficient is inversely proportional to the viscosity of the solution. Hence, any error in viscosity produces a corresponding error in the diffusion coefficient. Because results from relationships such as Eq. (6) can be considerably in error, experimental data should be used if they are available.

For HP-67/97 users

The HP program listing is contained in Table V, and Table VI offers user instructions. For the cyclohexane-benzene system example given for the TI program, Table VII summarizes the HP version results.

Program listing for HP version **Table V**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	036	GTO9	22 09	071	×	-35	106	÷	-24	141	ENT↑	-21
002	GSB8	23 08	037	*LBLC	21 13	072	1	01	107	√X	54	142	7	07
003	RCL0	36 00	038	GSB6	23 08	073	EEX	-23	108	÷	-24	143	÷	-24
004	RCL4	36 04	039	RCL0	36 00	074	CHS	-22	109	STO1	35 01	144	Yˣ	31
005	×	-35	040	√X	54	075	8	08	110	PRTX	-14	145	1	01
006	√X	54	041	×	-35	076	×	-35	111	R/S	51	146	+	-55
007		-35	042	RCL1	36 01	077	GTO9	22 09	112	RCL7	36 07	147	RCLC	36 13
008	RCL1	36 01	043	÷	-24	078	*LBLD	21 14	113	*LBLe	21 16 15	148	X⇄Y	-41
009	÷	-24	044	RCL2	36 02	079	STOE	35 [illegible]	114	SF0	16 21 00	149	Yˣ	31
010	RCL2	36 02	045	RCL3	36 03	080	R↓	-31	115	*LBLE	21 15	150	RCL8	36 08
011	.	-62	046	×	-35	081	STO7	35 07	116	STO6	35 06	151	×	-35
012	6	06	047	1	01	082	R↓	-31	117	STOB	35 12	152	F0?	16 23 00
013	Yˣ	31	048	ENT↑	-21	083	STO5	35 06	118	R↓	-31	153	GTO1	22 01
014	÷	-24	049	3	03	084	R↓	-31	119	STOC	35 13	154	STO2	35 02
015	7	07	050	÷	-24	085	STO3	35 03	120	R↓	-31	155	R/S	51
016	.	-62	051	Yˣ	31	086	RCL8	36 08	121	STOD	35 14	156	*LBL1	21 01
017	4	04	052	÷	-24	087	GSB6	23 09	122	R↓	-31	157	CF0	16 22 00
018	EEX	-23	053	STOA	35 11	088	STO8	35 08	123	STOE	35 15	158	STO3	35 03
019	CHS	-22	054	RCL3	36 03	089	*LBLd	21 16 14	124	8	08	159	R/S	51
020	8	08	055	RCL2	36 02	090	RCL6	36 06	125	2	02	160	*LBL8	21 08
021	×	-35	056	÷	-24	091	RCL8	36 08	126	.	-62	161	2	02
022	GTO9	22 09	057	1	01	092	÷	-24	127	0	00	162	7	07
023	*LBLB	21 12	058	.	-62	093	1	01	128	7	07	163	3	03
024	GSB8	23 06	059	5	05	094	−	-45	129	×	-35	164	.	-62
025	RCL9	36 09	060	X≤Y?	16-35	095	RCL7	36 07	130	RCLD	36 14	165	1	01
026	×	-35	061	GTOa	22 16 11	096	×	-35	131	÷	-24	166	6	06
027	RCL1	36 01	062	1	01	097	10ˣ	16 33	132	STO8	35 08	167	+	-55
028	÷	-24	063	0	00	098	8	08	133	RCLB	36 12	168	RTN	24
029	RCL2	36 02	064	GTO7	22 07	099	.	-62	134	GSB6	23 06	169	*LBL9	21 09
030	1	01	065	*LBLa	21 16 11	100	5	05	135	RCLE	36 15	170	PRTX	-14
031	ENT↑	-21	066	8	09	101	6	06	136	÷	-24	171	SPC	16-11
032	3	03	067	.	-62	102	9	09	137	CHS	-22	172	R/S	51
033	÷	-24	068	5	05	103	÷	-24	138	1	01			
034	Yˣ	31	069	*LBL7	21 07	104	RCL7	36 07	139	+	-55			
035	÷	-24	070	RCLA	36 11	105	RCL0	36 00	140	2	02			

User instructions for HP version **Table VI**

Clear flag 0	**CLF0**
For Wilke-Chang equation:	
M_B, solvent molecular weight	**STO 0**
ϕ, association factor	**STO 4**
Viscosity of solvent, cP	**STO 1**
V_A, solute molecular volume	**STO 2**
t, temperature, °C	Key **A**
Output will be diffusion coefficient, cm²/s	
For Scheibel equation:	
Viscosity of solvent cP	**STO 1**
V_A, solute molecular volume	**STO 2**
K, constant of Eq., (3)	**STO 9**
t, temperature, °C	Key **B**
Output will be diffusion coefficient, cm²/s	
For Reddy-Doraiswamy equation:	
M_B, solvent molecular weight	**STO 0**
Viscosity of solvent, cP	**STO 1**

(Continued) Table VI

V_A, solute molecular volume	**STO 2**
V_B, solvent molecular volume	**STO 3**
t, temperature, °C	Key **C**
Output will be diffusion coefficient, cm²/s	
If viscosities are not known, they may be obtained as follows:	
V_B, solvent molecular volume	**ENTER ↑**
T_c, solvent critical temperature, K	**ENTER ↑**
θ, Thomas constant (Eq. (6))	**ENTER ↑**
t, temperature, °C	**Key D**
Output will be viscosity in cP.	
If molecular volumes are not known, they may be obtained as follows:	
T_c, critical temperature, K	**ENTER ↑**
P_c, critical pressure, atm	**ENTER ↑**
Z_{RA} compressibility factor	**ENTER ↑**
t_b, boiling point, °C	Key **E** (for solute) Key **e** (for solvent)
Output will be molecular volume, cm³/g-mol.	

Comparison of calculated and experimental coefficient values for cyclohexane-benzene system, HP version **Table VII**

D°_{AB} values are in 10^{-5} cm^2/s

t, °C	Wilke-Chang	Scheebel	Reddy-Doraiswamy	Sanni et al.
25	1.47*	1.98*	1.93*	2.09
	2.33†	3.15†	3.07†	
40	1.91*	2.58*	2.51*	2.65
	2.79†	3.77†	3.68†	
60	2.49*	3.37*	3.29*	3.45
	3.47†	4.70†	4.58†	

*Experimental values of viscosity of benzene used in calculating diffusion coefficient.
†Viscosity values calculated via Eq. (6) used in calculating diffusion coefficient.

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Section IV
Fluid Flow

Program sizes control valves for liquids
Program sizes pipe and flare manifolds for compressible flow
Calculating two-phase pressure drop
Program predicts pressure drop for steam flow
Estimate heat-tracing requirements for pipelines
Estimate equivalent line lengths of pipe circuits
Program predicts pressure drop for gas flow across an orifice meter

Program sizes control valves for liquids

This HP-67/97 program calculates the sizing coefficient for control valves in liquid service, even in cases involving reducers, choked flow and laminar or transitional flow.

Jon F. Monsen, Jamesbury Corp.

☐ A correctly-sized control valve achieves a high quality of control at a reasonable cost. Too small a valve will not pass the required flow. Too large a valve will cost more than a correctly-sized smaller valve, and will not control the flow as well, because it will not use its full control range.

The procedure for sizing a control valve is:

1. Calculate the required valve sizing coefficient (C_v) based on process data and manufacturers' valve data.
2. Consult valve manufacturers' tables of C_v vs. valve size. Then select the smallest valve with a C_v rating greater than or equal to the required C_v.
3. Check to see that the reducers required to install the valve will not change the valve selection. Choose a new valve with a greater C_v if necessary.
4. Check to see that the flow through the valve is not choked (avoid choked flow if possible).

When the liquid flow is turbulent, and the effects of

The program uses this algorithm — **Table I**

Step	Equations and logic
1. Calculate $P_{1_{vlv}}$	$P_{1_{vlv}} = P_1 - \Delta P_{inlet\ reducer}$ $\Delta P_{inlet\ reducer} = \left[0.5\left(1 - \frac{d^2}{D^2}\right)^2 + 1 - \frac{d^4}{D^4}\right]\frac{q^2 G_f}{K_E d^4}$ ($P_1 \neq 0$ when choked-flow option included) ($\Delta P_{inlet\ reducer} \neq 0$ when reducer option included)
2. Calculate ΔP_{vlv}	$\Delta P_{vlv} = \Delta P_{sizing} - \Delta P_{reducers}$ $\Delta P_{reducers} = \left[1.5\left(1 - \frac{d^2}{D^2}\right)^2\right]\frac{q^2 G_f}{K_E d^4}$ ($\Delta P_{reducers} \neq 0$ when reducer option included)
3. Calculate ΔP If $P_1 \neq 0$ (choked-flow option)	$\Delta P_{T_{vlv}} =$ $F_L^2\left[P_{1_{vlv}} - P_v\left(0.96 - 0.28\sqrt{\frac{P_v}{P_c}}\right)\right]$ If $\Delta P_{vlv} > \Delta P_{T_{vlv}}$, then $\Delta P = \Delta P_{T_{vlv}}$ If $\Delta P_{vlv} \leq \Delta P_{T_{vlv}}$, then $\Delta P = \Delta P_{vlv}$
If $P_1 = 0$	$\Delta P = \Delta P_{vlv}$
4. Calculate $C_{v(turbulent)}$	$C_{v(turbulent)} = \frac{q}{K_D}\sqrt{\frac{G_f}{\Delta P}}$
5. Calculate C_v If $\mu \neq 0$ (laminar-flow option)	$F_s = \left[\frac{F_d^2}{F_L}\right]^{1/3}$ $C_{v(laminar)} = \frac{1}{F_s}\left[\frac{q\mu}{K_c \Delta P}\right]^{2/3}$ $F_R = 0.64 + 0.17 \ln \frac{C_{v(turbulent)}}{C_{v(laminar)}}$ If $F_R < 0.54$, then $C_v = C_{v(laminar)}$ If $0.54 \leq F_R < 1$, then $C_v = \frac{C_{v(turbulent)}}{F_R}$ If $F_R \geq 1$, then $C_v = C_{v(turbulent)}$
If $\mu = 0$	$C_v = C_{v(turbulent)}$
6. Display C_v	Stop here unless checking for choked flow
7. Check for choked flow If $P_1 = 0$	Display "ERROR"
If $P_1 \neq 0$ (choked-flow option)	$\Delta P_T = \Delta P_{T_{vlv}} + \Delta P_{reducers}$ If $\Delta P_{sizing} \leq \Delta P_T$, then display "0.00" (nonchoked) If $\Delta P_{sizing} > \Delta P_T$, then flow is choked If $P_v > P_1 - \Delta P_{sizing}$, then display "1.00" (flashing) If $P_v \leq P_1 - \Delta P_{sizing}$, then display "2.00" (cavitating)
8. Display ΔP_T	End

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choked flow and reducers are ignored, the expression for C_v reduces to:

$$C_v = \frac{q}{K_D}\sqrt{\frac{G_f}{\Delta P_{\text{sizing}}}}$$

This expression is so simple that its solution does not require a programmable calculator. But most installations do require reducers, and many situations demand that the designer check for flashing or cavitation in the valve. When these factors are considered, the calculations get very complicated. In such cases, a calculator program can simplify the task considerably.

What the program can do

In the simplest case, the program uses the above equation to calculate C_v. But the user has the option to check and correct for reducers, choked flow, and laminar or transitional flow. These options may be included or omitted in any combination, so the user can solve a problem as quickly as possible.

Table I shows the algorithm and equations used by

Nomenclature

C_v	Valve sizing coefficient
C_v (laminar)	Valve sizing coefficient when flow is fully laminar
C_v (turbulent)	Valve sizing coefficient when flow is fully turbulent
d	Nominal valve size
D	Internal diameter of the piping
F_d	Valve-style modifier
F_L	Rated liquid pressure-recovery factor (Table V)
F_R	Reynolds number factor
F_s	Laminar-flow factor
G_f	Specific gravity at flowing temperature
K_C, K_D, K_E	Constants stored on data card (Table II)
P_1	Absolute static pressure upstream of inlet reducer
$P_{1\ \text{vlv}}$	Absolute static pressure at valve inlet

Program listing for HP-67/97 calculator — **Table II**

Step	Key	Code
	Store data	
001	*LBLA	21 11
002	STO2	35 02
003	R↓	-31
004	STO0	35 00
005	R/S	51
006	*LBLa	21 16 11
007	STO1	35 01
008	R/S	51
009	*LBLB	21 12
010	STO3	35 03
011	R/S	51
012	*LBLb	21 16 12
013	STO8	35 08
014	R↓	-31
015	STO5	35 05
016	R↓	-31
017	STO4	35 04
018	R/S	51
019	*LBLC	21 13
020	STO7	35 07
021	R/S	51
022	*LBLc	21 16 13
023	STO6	35 06
024	R/S	51
025	*LBLD	21 14
026	STO8	35 08
027	R/S	51
028	*LBLd	21 16 14
029	STOA	35 11
030	R↓	-31
031	STO9	35 09
032	R/S	51
	Calculate $P_{1\ \text{vlv}}$	
033	*LBLE	21 15
034	1	01
035	RCL7	36 07

Step	Key	Code
036	RCL6	36 06
037	÷	-24
038	X^2	53
039	-	-45
040	X^2	53
041	2	02
042	÷	-24
043	1	01
044	+	-55
045	RCL7	36 07
046	RCL6	36 06
047	÷	-24
048	X^2	53
049	X^2	53
050	-	-45
051	RCL0	36 00
052	X^2	53
053	RCL1	36 01
054	x	-35
055	RCLE	36 15
056	÷	-24
057	RCL7	36 07
058	X^2	53
059	X^2	53
060	÷	-24
061	ENT↑	-21
062	R↓	-31
063	x	-35
064	CHS	-22
065	RCL3	36 03
066	+	-55
067	P⇄S	16-51
068	STO3	35 03
069	P⇄S	16-51
	Calculate $\Delta P_{T\ \text{vlv}}$	
070	R↑	16-31
071	1	01

Step	Key	Code
072	RCL7	36 07
073	RCL6	36 06
074	÷	-24
075	X^2	53
076	-	-45
077	X^2	53
078	1	01
079	.	-62
080	5	05
081	x	-35
082	x	-35
083	P⇄S	16-51
084	STO5	35 05
085	P⇄S	16-51
086	CHS	-22
087	RCL2	36 02
088	+	-55
089	P⇄S	16-51
090	STO2	35 02
091	P⇄S	16-51
	If P_1 = 0, skip choked-flow option	
092	RCL3	36 03
093	X=0?	16-43
094	GTO2	22 02
	Calculate ΔP_{vlv}	
095	P⇄S	16-51
096	RCL3	36 03
097	P⇄S	16-51
098	.	-62
099	9	09
100	6	06
101	RCL5	36 05
102	RCL4	36 04
103	÷	-24
104	$\sqrt{X}$	54
105	.	-62

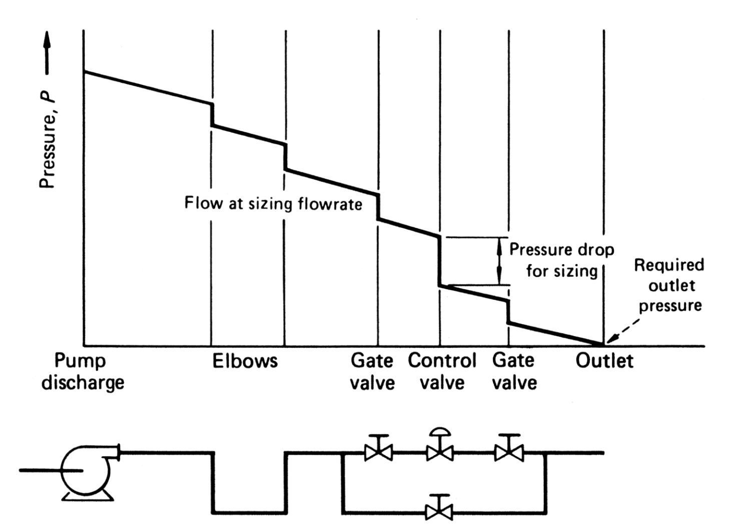
Step	Key	Code
106	2	02
107	8	08
108	x	-35
109	-	-45
110	RCL5	36 05
111	x	-35
112	-	-45
113	RCL8	36 08
114	X^2	53
115	x	-35
116	P⇄S	16-51
117	STO6	35 06
	ΔP = smaller of ΔP_{vlv} and $\Delta P_{T\ \text{vlv}}$	
118	RCL2	36 02
119	X≤Y?	16-35
120	GTO3	22 03
121	RCL6	36 06
122	*LBL3	21 03
123	STO4	35 04
	Calculate $C_{V\ (\text{turbulent})}$	
124	1/X	52
125	P⇄S	16-51
126	RCL1	36 01
127	x	-35
128	$\sqrt{X}$	54
129	RCL0	36 00
130	x	-35
131	RCLD	36 14
132	÷	-24
133	STOB	35 12
	If μ = 0, skip laminar-flow option	
134	RCLA	36 11
135	X=0?	16-43
136	GTO8	22 08

Step	Key	Code
	Calculate $C_{V\ (\text{laminar})}$	
137	RCL0	36 00
138	x	-35
139	RCLC	36 13
140	÷	-24
141	P⇄S	16-51
142	RCL4	36 04
143	P⇄S	16-51
144	÷	-24
145	X^2	53
146	3	03
147	1/X	52
148	Y^x	31
149	RCL9	36 09
150	X^2	53
151	RCL8	36 08
152	÷	-24
153	3	03
154	1/X	52
155	Y^x	31
156	÷	-24
	Calculate F_R	
157	÷	-24
158	ENT↑	-21
159	LN	32
160	.	-62
161	1	01
162	7	07
163	x	-35
164	.	-62
165	6	06
166	4	04
167	+	-55
168	.	-62
	Calculate C_V	
169	5	05
170	4	04

P_c	Thermodynamic critical pressure of liquid
P_v	Absolute vapor pressure of liquid at inlet temperature
ΔP	Pressure drop used in sizing equations
$\Delta P_{\text{inlet reducer}}$	Pressure drop due to inlet reducer
$\Delta P_{\text{reducers}}$	Combined pressure drop due to inlet and outlet reducers
ΔP_{sizing}	Pressure drop for sizing purposes across the valve-reducer combination
ΔP_T	Terminal or maximum pressure drop across the valve-reducer combination that allows nonchoked flow
$\Delta P_{T\ \text{vlv}}$	Terminal or maximum pressure drop across the valve that allows nonchoked flow
ΔP_{vlv}	Pressure drop across the valve
q	Volumetric flowrate
μ	Viscosity, cP

(Continued) Table II

Step	Key	Code	Step	Key	Code
171	X>Y?	16-34	202	GTO5	22 05
172	GTO7	22 07	203	RCL3	36 03
173	CLX	-51	204	RCL2	36 02
174	1	01	205	-	-45
175	X≤Y?	16-35	206	RCL5	36 05
176	GTO8	22 08	207	X≤Y?	16-35
177	R↓	-31	208	GTO6	22 06
178	1/X	52	209	1	01
179	RCLB	36 12	210	GTOe	22 16 15
180	×	-35	211	*LBL2	21 02
181	GTO9	22 09	212	P⇄S	16-51
182	*LBL8	21 08	213	RCL2	36 02
183	RCLB	36 12	214	GTO3	22 03
184	GTO9	22 09	215	*LBL5	21 05
185	*LBL7	21 07	216	0	00
186	RCLB	36 12	217	GTOe	22 16 15
187	R↑	16-31	218	*LBL6	21 06
188	÷	-24	219	2	02
189	*LBL9	21 09	220	GTOe	22 16 15
Error message if P_1 for			**Display coded message**		
choked-flow not entered			221	*LBLe	21 16 15
190	R/S	51	222	R/S	51
191	RCL3	36 03	223	RCLI	36 46
192	X=0?	16-43	224	R/S	51
193	GTO4	22 04	**Display ΔP_T**		
Calculate ΔP_T					
194	P⇄S	16-51			
195	RCL6	36 06			
196	RCL5	36 05			
197	+	-55			
198	STOI	35 46			
Determine whether flow is choked, and whether it is flashing or cavitating					
199	P⇄S	16-51			
200	RCL2	36 02			
201	X≤Y?	16-35			



Determine pressure drop for sizing by examining system pressure drops **Fig. 1**

Key principles

Pressure drop for sizing. The pressure drop used to size the control valve (ΔP_{sizing}) should not be an arbitrary number. In operation, the automatic control equipment will adjust the control-valve opening until the desired *flowrate* is achieved. The pressure drop used for sizing should be the actual pressure drop across the valve at the sizing flowrate.

Fig. 1 shows how to calculate ΔP_{sizing}: Start with the system pressure drop. Subtract from it the pressure drop at the sizing flowrate of all pipe, fittings and equipment in the flow system. The *remainder* is the actual pressure drop across the control valve at the sizing flowrate—this remainder is ΔP_{sizing}.

Choked flow. As the liquid passes the point of greatest restriction inside the control valve, its velocity reaches a maximum and its pressure falls to a minimum. If the pressure falls below the liquid's vapor pressure, vapor bubbles form within the valve. Increasing the pressure drop across the valve beyond the point where vapor bubbles form has no effect on the flow. Thus the flow is said to be choked. The pressure drop at which choked flow begins is referred to as terminal pressure drop (ΔP_T). When the actual pressure drop across the valve is greater than ΔP_T, ΔP_T should be used for the sizing calculation.

Flashing and cavitation. Choked flow produces either flashing or cavitation. If the pressure downstream of the valve is below the liquid's vapor pressure, the vapor bubbles persist in the liquid. This is flashing. Because the velocity of the flashing vapor-liquid stream is much higher than the inlet liquid velocity, the flashing stream often erodes valve internals or downstream piping. If, under choked-flow conditions, the downstream pressure is above the liquid's vapor pressure, the vapor bubbles will collapse as they leave the point of greatest restriction in the valve. This is cavitation. The shock waves and noise caused by the collapsing bubbles cause rapid and severe damage to the valve or piping.

the program. Though based on the ISA Standard [1], these equations solve for C_v directly instead of through an iterative technique. This saves time, and the result is the same. The approximation for laminar and transitional flow are based on [1] and [2].

How to use the program

Load the program as listed in Table II, and record it on a magnetic card. Store the constants listed in Table III in the specified registers and record them on a separate card (one set per side). The given constants are for the most often-used English and metric units—the user can develop constants for any other set of units. The program is now ready to go, and is stored on cards for easy future access. Table IV lists the user instructions for the program.

For the simplest case, enter the volumetric flowrate (q), the pressure drop for sizing (ΔP_{sizing}), and the specific gravity of the liquid at the inlet temperature (G_f). Then solve for C_v.

When the flow is not known to be turbulent (as is required in the simplest case), enter additional data to include laminar- or transitional-flow effects: pressure recovery factor (F_L) (Table V) for the type of valve being considered; valve style modifier (F_d); the viscosity of the liquid at the inlet temperature (μ). Then solve for C_v.

To include the effect of reducers, enter additional

Units and associated constants for data card — **Table III**

Variables	English units	Metric units
q	gal/min	m^3/h
ΔP (all subscripts)	psi	kPa
P (all subscripts)	psia	kPa abs
d, D	in.	mm
μ	cP	cP
Associated constants and locations		
K_C **(STO C)**	52.3	1.72
K_D **(STO D)**	1.0	0.0865
K_E **(STO E)**	890	1.6×10^{-5}
(STO 6)	1.0	1.0
(STO 7)	1.0	1.0
All other registers clear		

User instructions for program — **Table IV**

Step	Instructions	Input	Keys	Output
1	Load program (sides 1 and 2 of card)			
2	Load one side of data card (with desired units); this clears the registers			
3	Input data			
	Volumetric flowrate	q	↑	
	Pressure drop for sizing	ΔP_{sizing}	A	
	Specific gravity	G_f	f a	
	Choked-flow option only			
	Absolute pressure upstream of valve	P_1	B	
	Thermodynamic critical pressure	P_c	↑	
	Vapor pressure of fluid	P_v	↑	
	Pressure-recovery factor*	F_L	f b	
	Reducer option only			
	Nominal valve size	d	C	
	Inside diameter of pipe	D	f c	
	Laminar-flow option only			
	Pressure-recovery factor*	F_L	D	
	Valve-style modifier†	F_d	↑	
	Viscosity	μ	f d	
4	Solve for required C_v		E	C_v
5	Check for choked flow (only after solving for C_v and only if data for choked-flow option were entered)		R/S	0.00 if nonchoked 1.00 if flashing 2.00 if cavitating ERROR if no data
	Solve for terminal pressure drop		R/S	ΔP_T
6	To revise or add data, go back to Step 3			
7	For a new case, go back to Step 2			

*F_L is obtained from manufacturers' literature. Table V shows typical values.
†Use F_d = 1.0 for ball valves and single-ported globe valves; use F_d = 0.7 for valves with two parallel flowpaths, such as double-ported globe valves and butterfly valves. From [1].

Typical values for liquid pressure-recovery factor — **Table V**

Valve type	F_L
Single-seated globe, cage trim	0.86
Single-seated globe, contoured trim	0.86
Single-seated globe, cavitation-control cage trim	0.92
High-performance butterfly, 90° open	0.57
High-performance butterfly, 60° open	0.66
High-performance butterfly, 30° open	0.85
Ball, 90° open	0.45
Ball, 60° open	0.81
Ball, 30° open	0.95

data: nominal valve size (d), and inside diameter of inlet and outlet pipe (D). If the valve diameter is not known in advance, then (1) calculate C_v and choose the valve (ignoring the effect of reducers), (2) use the valve size from (1) to calculate the new C_v with reducers, and (3) check to see that the chosen valve can satisfy the new C_v requirement.

If ΔP_{sizing} is a significant part of upstream pressure, or if liquid vapor pressure is high, check and correct for choked flow. This requires more data: absolute pressure upstream of the valve (P_1); critical pressure of the fluid (P_c); vapor pressure of the fluid at the inlet temperature (P_v); and pressure-recovery factor (F_L). Solve for C_v, then press **R/S** to get a message that describes the flow through the valve: 0.00 for nonchoked; 1.00 for flashing; and 2.00 for cavitation. Press **R/S** again to get the terminal pressure drop (ΔP_T).

Note: Entering the data for any of the options automatically invokes those options. If the data are not entered, the program ignores those options. Checking for choked flow requires that the user hit the **R/S** key and that the correct data be entered. If the data are not entered, **R/S** will produce an error message instead of a coded message.

Examples

Case 1 (simplest case). Size a control valve for a liquid stream with: $q = 500$ gal/min; $\Delta P_{sizing} = 15$ psi; $G_f = 1.0$. Ignore reducers and the possibility of choked flow. Solution:

1. Load the program.
2. Load the side of the data card with English units.
3. Key in q, ΔP_{sizing}: 500 ↑ 15 **A**
4. Key in G_f: 1.0 **f a**
5. Solve for C_v: **E** 129.10
6. Choose a valve whose C_v is greater than or equal to 129.10.

Case 2 (possibility of choked flow; reducers). Size a globe-type control valve, given the following process data: $q = 400$ gal/min; $\Delta P_{sizing} = 20$ psi; $G_f = 0.98$; $P_1 = 50$ psia; $P_c = 3{,}206$ psia; $P_v = 2.9$ psia; $D = 6$ in. Manufacturers' literature (and Table V) shows $F_L = 0.86$ for a single-seated globe valve. Solution (assuming the program is still loaded):

1. Reload the side of the data card with English units.
2. Key in q, ΔP_{sizing}: 400 ↑ 20 **A**
3. Key in G_f: 0.98 **f a**
4. Key in P_1: 50 **B**
5. Key in P_c, P_v, F_L: 3,206 ↑ 2.9 ↑ 0.86 **f b**
6. Solve for C_v: **E** 88.54

Before choosing a valve, check for choked flow:

7. Check for choked flow: **R/S** 0.00
8. Solve for ΔP_T: **R/S** 34.94

The 0.00 display indicates that the flow is not choked (ΔP_{sizing} is less than ΔP_T). Checking the valve manufacturers' literature, one can find that a 3-in. globe valve with a maximum C_v rating of 120 is the smallest available valve with adequate C_v. To verify that the reducers required to install a 3-in. valve in a 6-in. line will not change the valve selection, continue as follows:

9. Key in d: 3 **C**
10. Key in D: 6 **f c**
11. Solve for C_v: **E** 92.91

Because the valve coefficient has changed, recheck the possibility of choked flow:

12. Check for choked flow: **R/S** 0.00
13. Solve for ΔP_T: **R/S** 34.81

Since C_v is still less than the maximum C_v rating of the chosen valve (120), and the flow is not choked, the 3-in. globe valve is the right choice.

Case 3 (laminar flow). Size a globe-type control valve, given the following process data: $q = 3$ m^3/h; $\Delta P_{sizing} = 35$ kPa; $G_f = 0.99$; $\mu = 300$ cP. Manufacturers' literature (and Table V) shows $F_L = 0.86$ for a single-seated globe valve. The user instructions in Table IV show $F_d = 1.0$ for a single-ported globe valve. Solution (assuming the program is still loaded):

1. Load the side of the data card with metric units
2. Key in q, ΔP_{sizing}: 3 ↑ 35 **A**
3. Key in G_f: 0.99 **f a**
4. Key in F_L: 0.86 **D**
5. Key in F_d, μ: 1.0 ↑ 300 **f d**
6. Solve for C_v: **E** 9.09
7. Choose a valve whose C_v is greater than or equal to 9.09.

For TI users

A listing of the program for the TI-58/59 is shown in Table VI. User instructions are listed in Table VII. The storage of constants follows as Table VIII.

As with the HP version, the calculation for C_v is obtained by pressing the **E** key. Then, pressing the **R/S** key solves for ΔP_T.

Program listing for TI version **Table VI**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	064	54	)	128	65	×	192	43	RCL	256	95	=
001	11	A	065	33	X^2	129	01	1	193	12	12	257	42	STO
002	42	STO	066	54	)	130	93	.	194	76	LBL	258	26	26
003	02	02	067	33	X^2	131	05	5	195	44	SUM	259	93	.
004	32	X↕T	068	55	÷	132	95	=	196	42	STO	260	06	6
005	42	STO	069	02	2	133	42	STO	197	14	14	261	04	4
006	00	00	070	85	+	134	15	15	198	53	(	262	85	+
007	91	R/S	071	01	1	135	94	+/-	199	35	1/X	263	93	.
008	76	LBL	072	75	-	136	85	+	200	65	×	264	01	1
009	16	A'	073	53	(	137	43	RCL	201	43	RCL	265	07	7
010	42	STO	074	43	RCL	138	02	02	202	01	01	266	65	×
011	01	01	075	07	07	139	95	=	203	54	)	267	53	(
012	91	R/S	076	55	÷	140	42	STO	204	34	√X	268	53	(
013	76	LBL	077	43	RCL	141	12	12	205	65	×	269	43	RCL
014	12	B	078	06	06	142	00	0	206	43	RCL	270	21	21
015	42	STO	079	54	)	143	32	X↕T	207	00	00	271	55	÷
016	04	04	080	45	Y^x	144	43	RCL	208	55	÷	272	43	RCL
017	32	X↕T	081	04	4	145	03	03	209	43	RCL	273	26	26
018	42	STO	082	54	)	146	67	EQ	210	23	23	274	54	)
019	03	03	083	65	×	147	24	CE	211	95	=	275	23	LNX
020	91	R/S	084	53	(	148	53	(	212	42	STO	276	54	)
021	76	LBL	085	53	(	149	43	RCL	213	21	21	277	95	=
022	17	B'	086	43	RCL	150	13	13	214	00	0	278	42	STO
023	42	STO	087	00	00	151	75	-	215	32	X↕T	279	27	27
024	08	08	088	33	X^2	152	43	RCL	216	43	RCL	280	01	1
025	32	X↕T	089	65	×	153	05	05	217	20	20	281	32	X↕T
026	42	STO	090	43	RCL	154	65	×	218	67	EQ	282	43	RCL
027	05	05	091	01	01	155	53	(	219	33	X^2	283	27	27
028	91	R/S	092	55	÷	156	93	.	220	53	(	284	77	GE
029	76	LBL	093	43	RCL	157	09	9	221	43	RCL	285	33	X^2
030	13	C	094	24	24	158	06	6	222	20	20	286	93	.
031	42	STO	095	55	÷	159	75	-	223	65	×	287	05	5
032	07	07	096	43	RCL	160	93	.	224	43	RCL	288	04	4
033	91	R/S	097	07	07	161	02	2	225	00	00	289	32	X↕T
034	76	LBL	098	45	Y^x	162	08	8	226	55	÷	290	43	RCL
035	18	C'	099	04	4	163	65	×	227	43	RCL	291	27	27
036	42	STO	100	54	)	164	53	(	228	22	22	292	77	GE
037	06	06	101	42	STO	165	43	RCL	229	55	÷	293	34	√X
038	91	R/S	102	26	26	166	05	05	230	43	RCL	294	43	RCL
039	76	LBL	103	54	)	167	55	÷	231	02	02	295	26	26
040	14	D	104	94	+/-	168	43	RCL	232	54	)	296	61	GTO
041	42	STO	105	85	+	169	04	04	233	45	Y^x	297	35	1/X
042	08	08	106	43	RCL	170	54	)	234	53	(	298	76	LBL
043	91	R/S	107	03	03	171	34	√X	235	02	2	299	33	X^2
044	76	LBL	108	95	=	172	54	)	236	55	÷	300	43	RCL
045	19	D'	109	42	STO	173	54	)	237	03	3	301	21	21
046	42	STO	110	13	13	174	65	×	238	54	)	302	61	GTO
047	20	20	111	43	RCL	175	43	RCL	239	55	÷	303	35	1/X
048	32	X↕T	112	26	26	176	08	08	240	53	(	304	76	LBL
049	42	STO	113	65	×	177	33	X^2	241	53	(	305	34	√X
050	09	09	114	53	(	178	95	=	242	43	RCL	306	43	RCL
051	91	R/S	115	01	1	179	42	STO	243	09	09	307	21	21
052	76	LBL	116	75	-	180	16	16	244	33	X^2	308	55	÷
053	15	E	117	53	(	181	43	RCL	245	55	÷	309	43	RCL
054	53	(	118	43	RCL	182	12	12	246	43	RCL	310	27	27
055	53	(	119	07	07	183	32	X↕T	247	08	08	311	95	=
056	01	1	120	55	÷	184	43	RCL	248	54	)	312	76	LBL
057	75	-	121	43	RCL	185	16	16	249	45	Y^x	313	35	1/X
058	53	(	122	06	06	186	77	GE	250	53	(	314	99	PRT
059	43	RCL	123	54	)	187	23	LNX	251	01	1	315	91	R/S
060	07	07	124	33	X^2	188	61	GTO	252	55	÷	316	61	GTO
061	55	÷	125	54	)	189	44	SUM	253	03	3	317	43	RCL
062	43	RCL	126	33	X^2	190	76	LBL	254	54	)			
063	06	06	127	95	=	191	23	LNX	255	54	)			

(Continued) Table VI

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
318	76	LBL	330	67	EQ	342	25	25	354	77	GE	366	02	2
319	24	CE	331	54	)	343	77	GE	355	52	EE	367	76	LBL
320	43	RCL	332	43	RCL	344	45	Y^x	356	01	1	368	53	(
321	12	12	333	02	02	345	43	RCL	357	61	GTO	369	19	D'
322	61	GTO	334	32	X:T	346	05	05	358	53	(	370	44	SUM
323	23	LNX	335	43	RCL	347	32	X:T	359	76	LBL	371	25	25
324	76	LBL	336	15	15	348	43	RCL	360	45	Y^x	372	99	PRT
325	43	RCL	337	85	+	349	03	03	361	00	0	373	91	R/S
326	00	0	338	43	RCL	350	75	-	362	61	GTO			
327	32	X:T	339	16	16	351	43	RCL	363	53	(			
328	43	RCL	340	95	=	352	02	02	364	76	LBL			
329	03	03	341	42	STO	353	95	=	365	52	EE			

User instructions for TI program **Table VII**

Step	Procedure	Input	Key	Output
1.	Load program			
2.	Store constants (See Table VIII)			
3.	Input data:			
	a. Case 1	q	x⇄t	
		ΔP	A	
		G_f	A'	
		—	E	C_v
	b. Case 2: Same as case 1 plus additional data (repeat steps 3a.)	P_1	x⇄t	
		P_c	B	
		P_v	x⇄t	
		F_L	B'	
			E	C_v
			R/S	Choke?
				ΔP_T
	c. Case 2 with reducers: Same as case 2 plus (repeat steps 3a., 3b.)	d	C	
		D	C'	
			E	C_v
			R/S	Choke?
				ΔP_T
	d. Case 3: Same as case 1 plus (repeat step 3a.)	F_L	D	
		F_d	x⇄t	
		μ	D'	

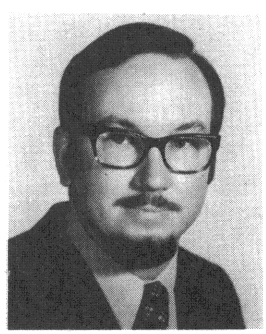
Storage of constants for TI program **Table VIII**

Register	English Units	Metric Units
STO 06	1	1
STO 07	1	1
STO 22	52.3	1.72
STO 23	1	0.0865
STO 24	890	0.000016

References

1. "ANSI/ISA-S75.01 Standard Control Valve Sizing Equations," Instrument Soc. of America, Pittsburgh, 1978.
2. Driskell, L. R., Sizing Control Valves, Chapter 6 of "ISA Handbook of Control Valves," Instrument Soc. of America, Pittsburgh, 1976.
3. "Engineering Handbook for Jamesbury Stabilflo Control Valves," Bulletin 275, Jamesbury Corp., 1980.

The author



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Program sizes pipe and flare manifolds for compressible flow

Written for the TI-58 or TI-59, this program sizes pipe for isothermal flow. Conditions can be calculated at pipe inlets or outlets.

Paul Kandell, *PEDCo, Inc.*

☐ In sizing pipe for the flow of liquids, the Darcy, or Fanning, equation is usually used. Such methods may also be used for the flow of gases within certain restricted ranges (for details on these ranges, see Ref. [*1*]). However, in the design of process plants, compressible flow is usually encountered, with its characteristic rapid changes in density and velocity. Other equations are needed for compressible flow.

Lapple [*2*] lists these for isothermal and adiabatic flow. Others present simplified forms of these expressions that have restrictive assumptions. Some empirical equations designed for limited use, such as the Weymouth and Panhandle formulae, appear in Ref. [*1*].

Typical of the compressible-flow design problems in chemical process plants and refineries is sizing pressure-relief manifold systems. In such systems, it is necessary to calculate the backpressure (the pressure in the header) developed at relief valve outlets when these are relieving concurrently. If the backpressure gets too high, some of the closed valves may not open at their proper pressures. For example, ordinary relief valves tolerate variable backpressures to 10% of the valve set pressure. Balanced-bellows relief valves can be used for backpressures to 30—50% of the set pressure, above which their capacities decrease.

Conventional equations

Many methods based on isothermal flow have been proposed for sizing relief headers (and, of course, process piping). Most notable are those methods given in API RP-520, Part 1 [*3*], which has a kinetic-energy correction factor, and in API RP-521 [*4*] which is based on the Lapple chart. An inherent difficulty in these methods is that they are based on the header inlet or backpressure, which is unknown. Backpressure is unknown since, at any relief-valve outlet, it depends on the flows of other valves discharging simultaneously into the same relief manifold.

Therefore, all of these methods require a tedious trial-and-error solution based on an assumed inlet pressure. In a refinery, for example, if cooling water or power fails, there may be a large number of relief valves, perhaps as many as ten, concurrently discharging into the same relief header. The problems posed by these manual trial-and-error solutions can be hopelessly complicated.

Calculations can be simplified by using graphic solutions [*5,6,7*]. These, however, are not convenient or flexible enough for general use, say in sizing gas-transmission pipelines, or in situations that have large pressure drops.

Here, we will present a streamlined calculation method that can solve a formidable array of compressible-flow problems.

The calculator program

The accompanying program, designed for the TI-58 and TI-59 calculators, does solve a broad range of pipe-sizing problems for compressible flow. The program assumes that flow is isothermal, and that either the upstream pressure or the downstream pressure is known. The Mach number can be found at the inlet and, more importantly, at the outlet—where sonic velocity may limit the flow.

The program has been deliberately economized to fit the storage capacity of the TI-58, since this model is widely used by young design engineers.

The program is listed in Table I and the user instructions are given in Table II.

The algorithm

Isothermal conditions, based on the inlet pressure, can be expressed as [*2*]:

$$fL/D = (1/M_1^2)[1 - (P_2/P_1)^2] - \ln(P_1/P_2)^2 \quad (1)$$

If we let r equal the ratio of P_1 to P_2, then:

$$r^2 = r^2M_1^2(fL/D + \ln r^2) + 1 \quad (2)$$

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Program listing for compressible flow of fluids **Table I**

Location	Code	Key
Enters P_2; sets flag		
000	76	LBL
001	12	B
002	42	STO
003	12	12
004	86	STF
005	00	00
006	91	R/S
Enters P_1; clears flag		
007	76	LBL
008	13	C
009	42	STO
010	12	12
011	22	INV
012	86	STF
013	00	00
014	91	R/S
Enters D and initializes program		
015	76	LBL
016	11	A
017	42	STO
018	14	14
Calc. A		
019	43	RCL
020	14	14
021	33	X²
022	65	×
023	89	π
024	55	÷
025	04	4
026	95	=
027	42	STO
028	15	15
Calc. W/P		
029	43	RCL
030	01	01
031	55	÷
032	43	RCL
033	12	12
034	95	=
035	42	STO
036	16	16
Calculate $[ZT/M_w]^{1/2}$		
037	53	(
038	43	RCL
039	07	07
040	65	×
041	43	RCL
042	02	02
043	55	÷
044	43	RCL
045	05	05
046	54	)
047	34	√X
048	42	STO
049	17	.17
Calc. M		
050	43	RCL
051	08	08
052	65	×
053	43	RCL
054	16	16
055	55	÷
056	43	RCL
057	15	15
058	65	×
059	43	RCL
060	17	17
061	95	=
062	42	STO
063	18	18
064	91	R/S
Calc. N_{Re}		
065	43	RCL
066	01	01
067	55	÷
068	43	RCL
069	15	15
070	95	=
071	42	STO
072	19	19
073	43	RCL
074	14	14
075	65	×
076	43	RCL
077	19	19
078	55	÷
079	43	RCL
080	03	03
081	95	=
082	42	STO
083	20	20
084	91	R/S
Calc. f		
085	43	RCL
086	06	06
087	55	÷
088	43	RCL
089	10	10
090	65	×
091	43	RCL
092	14	14
093	35	1/X
094	95	=
095	42	STO
096	21	21
097	43	RCL
098	11	11
099	55	÷
100	43	RCL
101	20	20
102	95	=
103	42	STO
104	22	22
105	04	4
106	42	STO
107	09	09
108	01	1
109	42	STO
110	23	23
111	76	LBL
112	15	E
113	53	(
114	43	RCL
115	21	21
116	85	+
117	43	RCL
118	22	22
119	65	×
120	43	RCL
121	23	23
122	34	√X
123	35	1/X
124	54	)
125	28	LOG
126	65	×
127	02	2
128	94	+/-
129	95	=
130	35	1/X
131	33	X²
132	42	STO
133	23	23
134	97	DSZ
135	09	09
136	15	E
137	91	R/S
Calc. fL/D		
138	43	RCL
139	23	23
140	65	×
141	43	RCL
142	04	04
143	55	÷
144	43	RCL
145	14	14
146	95	=
147	42	STO
148	24	24
Calc. r^2		
149	01	1
150	42	STO
151	25	25
152	76	LBL
153	16	A'
154	43	RCL
155	18	18
156	33	X²
157	65	×
158	53	(
159	43	RCL
160	24	24
161	85	+
162	43	RCL
163	25	25
164	23	LNX
165	54	)
166	87	IFF
167	00	00
168	17	B'
169	65	×
170	43	RCL
171	25	25
172	76	LBL
173	17	B'
174	85	+
175	01	1
176	95	=
177	52	EE
178	58	FIX
179	02	02
180	32	X⇌T
181	43	RCL
182	25	25
183	67	EQ
184	19	D'
185	32	X⇌T
186	42	STO
187	25	25
Calc. r		
188	61	GTO
189	16	A'
190	76	LBL
191	19	D'
192	22	INV
193	52	EE
194	58	FIX
195	09	09
196	34	√X
197	42	STO
198	26	26
Calc. P_2		
199	87	IFF
200	00	00
201	18	C'
202	43	RCL
203	12	12
204	55	÷
205	43	RCL
206	26	26
207	95	=
208	91	R/S
209	42	STO
210	13	13
Calc. P_1		
211	71	SBR
212	14	D
213	76	LBL
214	18	C'
215	43	RCL
216	12	12
217	65	×
218	43	RCL
219	26	26
220	95	=
221	91	R/S
222	42	STO
223	13	13
Calc. ΔP		
224	71	SBR
225	14	D
226	76	LBL
227	14	D
228	43	RCL
229	13	13
230	75	-
231	43	RCL
232	12	12
233	95	=
234	50	I×I
235	91	R/S
Retrieves P_1 or P_2		
236	43	RCL
237	13	13
238	91	R/S
239	81	RST

Nomenclature

A	Pipe internal cross-sectional area, ft²
D	Pipe ID, ft
d	Pipe ID, in.
f	Darcy friction factor
G	Mass velocity, lb/hr-sq ft
g_c	Gravitational constant, 32.17 lb-ft/lb$_f$-s²
k	Ratio of heat capacity at constant pressure to capacity at constant volume
L	Equivalent length, ft
M_1	Mach number at pipe inlet
M_2	Mach number at pipe outlet
M_w	Molecular weight of gas
MABP	Maximum allowable backpressure, psia
N_{Re}	Reynolds number
P_1	Pipe inlet pressure, psia

Also, if M_2 is the Mach number at the outlet, then, since $rM_1 = M_2$:

$$r^2 = M_2^2(fL/D + \ln r^2) + 1 \qquad (3)$$

In this program, the Mach number is calculated from the ratio of the actual velocity to the sonic velocity, which is in turn calculated from the equation [*5,8*]:

$$v_s = \left[\frac{g_c kRT}{M_w}\right]^{1/2} \qquad (4)$$

This equation reduces to:

$$v_s = 223\left[\frac{T}{M_w}\right]^{1/2} \qquad (5)$$

The actual velocity can be expressed as:

$$v_a = \frac{W}{\rho A}$$

and, since for actual gases, from the gas law:

$$\rho = \frac{PM_w}{ZRT}$$

then,

$$v_a = \left[\frac{W}{A}\right]\left[\frac{ZRT}{PM_w}\right] \qquad (6)$$

Combining Eq. (5) and (6), reducing to consistent units and simplifying, we have the Mach number:

$$M = 0.00001336\left[\frac{W}{PA}\right]\left[\frac{ZT}{M_w}\right]^{1/2} \qquad (7)$$

Since Eq. (2) and (3) are implicit in r, r^2 is calculated by assuming $r^2 = 1$ and looping the program until r^2_{actual} equals $r^2_{assumed}$.

Speeding convergence

It has been found, however, that in calculations where the ΔP was comparatively high, convergence was slow, especially in calculating P_2. The calculation sometimes took twenty minutes to complete. However, using

P_2	Pipe outlet pressure, psia
p_{set}	Relief valve set pressure, psig
R	Gas law constant, 1,543 ft-lb$_f$/°R-lb mol
r	Ratio of P_2 to P_1
T	Absolute temperature, °R
v_a	Actual velocity, ft/s
v_s	Sonic velocity, ft/s
W	Gas flowrate, lb/h
x	Mol fraction
Z	Gas compressibility factor
ε	Absolute roughness, ft (0.00015 for carbon steel pipe)
ρ	Density, lb/ft^3
μ	Viscosity in cP $\times$ 2.42 = lb/ft-h

the Newton-Raphson convergence to ± 0.001 gave sufficient accuracy, without unduly delaying the calculation; it took approximately two minutes for the most extreme and unusual case. Therefore, the development of a more rapidly converging algorithm, which adds steps to the program, was not justified.

The Darcy friction factor, f, is calculated from the Colebrook equation [*9*] which is the origin of the Moody chart [*10*]. The equation can be expressed as:

$$\frac{1}{\sqrt{f}} = -2 \log \left[\frac{\varepsilon}{3.7D} + \frac{2.51}{N_{Re}\sqrt{f}} \right] \quad (8)$$

This equation is implicit in f. By assuming $\sqrt{f} = 1$ and solving by trial and error, using Newton-Raphson convergence to ± 0.00001 [*11*], the friction factor can be calculated in four iterations to sufficient precision.

In the execution of this program, either P_2 or P_1 is entered. A pipe size, D, is then assumed and entered. For example, if P_2 is known and P_1 is sought, P_2 is entered and a pipe size is assumed. The program will then calculate M_2 (the Mach number associated with the entered pressure), followed by the Reynolds number, the Darcy friction factor, P_1, and finally the ΔP.

If the calculated M_2 is greater than 0.7, the outlet velocity is too close to sonic and the assumed pipe size is too small. Such a design will result in undue vibration and unacceptable noise generation. A larger pipe size is then assumed and the program run again until the Mach number at the pipe outlet is less than 0.7.

If P_1 is known and P_2 is sought, the procedure is similar except that the first calculated Mach number will be M_1. Since the criterion for pipe sizing is M_2, the program is continued until P_2 is displayed. Pressing the **R/S** button will display ΔP and pressing it again will retrieve P_2 into the display. This value may then be entered by pressing **B,** and the pipe diameter, D, is reentered directly or by recalling register 14 **(RCL 14).** M_2 will then be displayed at the first **R/S.** This, again, should be less than 0.7, or a larger pipe size must be assumed and the procedure repeated. Some problems will illustrate the method.

User's instructions. Inlet and outlet conditions may be obtained easily **Table II**

Step	Procedure	Enter	Press	Display
1.	Clear program memory		**2nd CP**	
2.	Enter learn mode		**LRN**	000 00
3.	Enter program			
4.	Exit learn mode		**LRN**	0
5.	Enter stored data:			
	W, lb/h	W	**STO 01**	W
	T, °R	T	**STO 02**	T
	μ, lb/ft-h	cP×2.42	**STO 03**	μ
	L, ft	L	**STO 04**	L
	M_w	M_w	**STO 05**	M_w
	ϵ, ft	(0.00015 for CS pipe)	**STO 06**	0.00015
	Z	Z	**STO 07**	Z
	Factor in Mach number	0.00001336	**STO 08**	0.00001336
	Constant in Colebrook equation	3.7	**STO 10***	3.7
	Constant in Colebrook equation	2.51	**STO 11**	2.51
6.	Enter P_1 or P_2 as independent variable	P_1 or P_2	**C** **B**	P_1 or P_2
7.	Enter D, ft, and initialize:	$D \div 12$	**A**	
	Read M_1 if P_1 entered, M_2 if P_2 entered		**R/S**	M_1 or M_2
	Read Reynolds number		**R/S**	N_{Re}
	Read Darcy friction factor		**R/S**	f
	Read P_2 if P_1 entered, P_1 if P_2 entered	Dependent variable	**R/S**	P_2 or P_1
	Read ΔP		**R/S**	ΔP
8.	Retrieve dependent variable (P_2 or P_1)		**R/S**	P_2 or P_1
9.	Enter displayed dependent variable	P_2 or P_1	**B** **C**	P_2 or P_1
10.	Reenter D (**RCL 14** or enter directly)	D	**A**	
11.	Read missing M at first R/S (M_2 for P_2 or M_1 for P_1 entered in Step 9)		**R/S**	M_2 or M_1

***Reg 09** is reserved for f iteration.

Sample problems

Example 1: What is the pressure drop and the outlet Mach number in a 12-inch, Sch. 30 pipeline, 800 ft long, with carbon dioxide flowing under the following conditions:

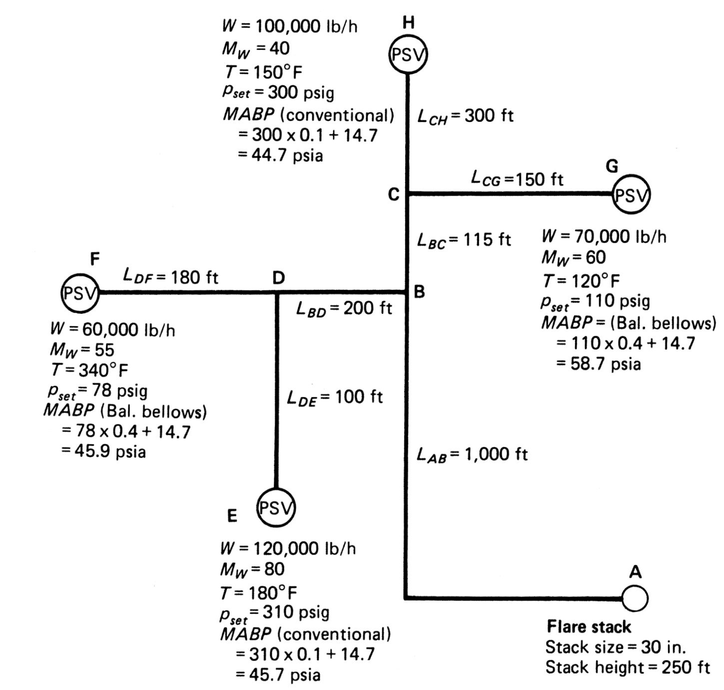
W = 250,000 lb/h
P_1 = 80 psia
T = 600°R
μ = 0.0167 cP $\times$ 2.42 = 0.040414 lb/ft-h
L = 800 ft
M_w = 44
Z = 1
D = 12.09 in. $\div$ 12 = 1.0075 ft

Data and results for Example 3. Such complex cases are worked out relatively quickly **Table III**

Line	Stack	AB	BD	DF	DE	BC	CH	CG
Nominal size, in.	30	18	12	8	8	12	10	6
Schedule	10	20	40	40	40	40	40	40
D, ft	2.448	1.448	0.9965	0.6651	0.6651	0.9965	0.8350	0.5054
L, ft	250	1,000	200	180	100	115	300	150
W, lb/h	350,000	350,000	180,000	60,000	120,000	170,000	100,000	70,000
T, °R	646.6	646.6	693.3	800	640	597.6	610	580
M_W	56	56	69.5	55	80	46.4	40	60
μ, lb/ft-h	0.0261	0.0261	0.0285	0.0315	0.0267	0.0240	0.0242	0.0237
MABP, psia	--	--	--	45.9	45.7	--	44.7	58.7
P_2, psia	atm.	15.1346	34.1452	37.8689	37.8689	34.1452	36.6166	36.6166
Calculated values								
M_2	0.2297	0.6375	0.2852	0.2324	0.3447	0.3061	0.2602	0.3958
N_{Re}	6,974,711	11,791,501	8,069,757	3,646,396	8,603,856	9,050,456	6,300,983	7,440,885
f	0.01132	0.01222	0.01314	0.01434	0.01419	0.01312	0.01362	0.01501
P_1	15.1346	34.1452	36.8689	41.8276	42.8438	36.6166	42.5446	48.9897
ΔP	0.4346	19.0106	3.7234	3.9587	4.9749	2.4714	5.9280	12.3731

The program calculates the following results:

$M_1 = 0.1933863318$
$N_{Re} = 7{,}817{,}596.221$
$f = 0.0131145068$
$P_2 = 61.53846154$
$\Delta P = 18.46153846$



The program makes the task of sizing a flare manifold much easier and less tedious

Then by retrieving P_2, entering the displayed value of P_2 by pressing **B**, reentering the diameter, D (or **RCL 14**) and reinitializing with **A**, we obtain at the first **R/S:**

$$M_2 = 0.2514022314$$

which indicates subsonic flow, and that the solution is acceptable.

Example 2: What is the pressure drop and the outlet Mach number for natural gas flowing through 3/4-in., Sch. 160 pipe under the following conditions:

$W = 8{,}380$ lb/h
$P_1 = 1{,}124.7$ psia
$T = 560$°R
$\mu = 0.01$ cP $\times 2.42 = 0.0242$ lb/ft-h
$L = 23$ ft
$M_w = 18.7$
$Z = 0.9$
$D = 0.614$ in. $\div 12 = 0.05117$ ft

The program calculates the following:

$M_1 = 0.2512971315$
$N_{Re} = 8{,}616{,}350.445$
$f = 0.0260122702$
$P_2 = 415.7010817$
$\Delta P = 708.9989183$

Then, by retrieving P_2 into the display by pressing **R/S**, entering the displayed value by pressing **B**, reentering the diameter directly (or by **RCL 14**) and reinitializing by pressing **A**, we obtain:

$$M_2 = 0.6798969169$$

which is less than 1.0, and therefore the flow is subsonic.

This problem illustrates the time to calculate P_2 under conditions of high pressure drop. In this case, with a ΔP of about 709 psi and a Mach number at the outlet of nearly 0.7, the calculation takes two minutes and twenty seconds on the TI-58, which is about the maximum calculation time encountered. Longer calculations should be manually terminated and rerun with a larger pipe size. This is accomplished by pressing **R/S** followed by **INV FIX.** Most problems encountered compute P_2 in less than ten seconds.

Sizing flare manifolds

Here are points to remember in sizing manifolds:

1. The design starts at the flare tip, where the outlet pressure is atmospheric. The calculation is worked backward toward the relief valves.
2. A size is assumed for each pipe section of the same diameter, and an equivalent length established.
3. The maximum allowed velocity at each section outlet is Mach 0.7.
4. Properties in the common headers may be estimated from the following mixture relationships (i indicates the ith component):

$$M_w = \Sigma W_i / \Sigma (W/M_w)_i \qquad (9)$$

$$T = \Sigma W_i T_i / \Sigma W_i \qquad (10)$$

$$\mu = \Sigma x_i \mu_i (M_w)_i^{0.5} / \Sigma x_i (M_w)_i^{0.5} \qquad (11)$$

5. The inlet pressure is calculated for each section of the line.
6. At each line size change, the inlet pressure for the downstream line (P_1) is taken as the outlet pressure of the upstream line (P_2) and a new upstream pressure (P_1) calculated.
7. The operation is repeated, working backward toward the relief valve.
8. The calculated backpressure at the relief valve is then checked against the maximum allowable backpressure (MABP). The calculated backpressure should be less than, but close to, the MABP.
9. The MABP is taken as 40% of the set pressure for balanced-bellows relief valves, and 10% of the set pressure for conventional relief valves.
10. If there is a great difference between the calculated backpressure and the MABP, the longest header should be decreased in size until the calculated backpressure is close to the MABP.

Example 3: Size the flare manifold with relief loads and flow conditions shown in the figure. For simplicity, the knockout drum is not shown.

This is the same problem solved graphically by Mak [6], and is presented here to demonstrate the simplicity of the method.

Table III summarizes the calculations. Note that the backpressures are close to, but less than, the MABPs, showing that the line sizing is acceptable.

Although many combinations of sizes are possible, good judgment would dictate minimizing the capital cost. The main header AB, which is 1,000 ft long, should be as small in diameter as possible.

Validity of the method

Finally, let us examine the validity of the use of the isothermal flow equation as opposed to the adiabatic flow equation. (Note that Mak [6] also deals with this problem.) Compared to adiabatic flow:

1. The isothermal equation yields a higher backpressure for both subsonic and sonic flow.
2. In subsonic flow, the maximum backpressure difference is less than 8%.
3. In sonic flow, the difference is less than 20% when fL/D is greater than 0.1.
4. Although the difference is greater than 20% for fL/D less than 0.1, this is academic, as such low values are rarely encountered.
5. The difference in backpressure is less than 4% when fL/D is greater than 10 for subsonic and sonic flows.

These deviations represent maximums of the calculated backpressure difference between the isothermal and the adiabatic equations. Actual flow in pipelines and relief systems normally takes place somewhere between adiabatic and isothermal conditions, and the deviation from the true value is greatly reduced.

Conclusion

This method provides a simple and rapid solution to an otherwise complex problem. Moreover, application of the program provides conservative values for backpressure, making it ideal for use in design of flare system manifolds and piping.

For HP-67/97 users

The HP version closely follows the TI program. Table IV contains the HP program listing, and user instructions all offered in Table V.

Program listing for HP version **Table IV**

Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	028	RCL1	36 01
002	STO4	35 04	029	×	-35
003	R↓	-31	030	RCL8	36 08
004	STO3	35 03	031	÷	-24
005	R↓	-31	032	RCL6	36 06
006	STO2	35 02	033	X²	53
007	R↓	-31	034	Pi	16-24
008	STO1	35 01	035	×	-35
009	R/S	51	036	4	04
010	STO6	35 06	037	÷	-24
011	R↓	-31	038	STO9	35 09
012	STO7	35 07	039	÷	-24
013	R↓	-31	040	RCL7	36 07
014	STO5	35 05	041	RCL2	36 02
015	R/S	51	042	×	-35
016	*LBLB	21 12	043	RCL5	36 05
017	SF1	16 21 01	044	÷	-24
018	*LBLC	21 13	045	√X	54
019	STO8	35 08	046	×	-35
020	1	01	047	PRTX	-14
021	.	-62	048	STOA	35 11
022	3	03	049	RCL1	36 01
023	3	03	050	RCL9	36 09
024	6	06	051	÷	-24
025	EEX	-23	052	RCL6	36 06
026	5	05	053	×	-35
027	CHS	-22	054	RCL3	36 03

(Continued) Table IV

Step	Key	Code	Step	Key	Code
055	÷	-24	099	÷	-24
056	PRTX	-14	100	RCLE	36 15
057	STOB	35 12	101	LN	32
058	4	04	102	+	-55
059	STOI	35 46	103	RCLA	36 11
060	1	01	104	X²	53
061	STOC	35 13	105	×	-35
062	*LBL6	21 06	106	F1?	16 23 01
063	RCLC	36 13	107	GTO8	22 08
064	√X	54	108	RCLE	36 15
065	1/X	52	109	×	-35
066	2	02	110	*LBL8	21 08
067	.	-62	111	1	01
068	5	05	112	+	-55
069	1	01	113	DSP2	-63 02
070	×	-35	114	RND	16 24
071	RCLB	36 12	115	STO8	35 08
072	÷	-24	116	RCLE	36 15
073	RCLD	36 14	117	X=Y?	16-33
074	3	03	118	GTO1	22 01
075	.	-62	119	RCL0	36 00
076	7	07	120	STOE	35 15
077	÷	-24	121	GTO7	22 07
078	RCL6	36 06	122	*LBL1	21 01
079	÷	-24	123	DSP9	-63 09
080	+	-55	124	RCLE	36 15
081	LOG	16 32	125	√X	54
082	2	02	126	RCL8	36 08
083	×	-35	127	F1?	16 23 01
084	CHS	-22	128	GTO2	22 02
085	1/X	52	129	X⇄Y	-41
086	X²	53	130	÷	-24
087	STOC	35 13	131	GTO3	22 03
088	DSZI	16 25 46	132	*LBL2	21 02
089	GTO6	22 06	133	×	-35
090	PRTX	-14	134	*LBL3	21 03
091	STOC	35 13	135	PRTX	-14
092	1	01	136	RCL8	36 08
093	STOE	35 15	137	-	-45
094	*LBL7	21 07	138	ABS	16 31
095	RCLC	36 13	139	PRTX	-14
096	RCL4	36 04	140	CF1	16 22 01
097	×	-35	141	R/S	51
098	RCL6	36 06			

User instructions for HP version **Table V**

Step	Procedure	Key
1.	Clear flag 1.	F CLF 1
2.	Enter program manually, or from both sides of a magnetic card.	
3.	Store absolute roughness in register D; i.e., 0.00015 (for carbon steel pipe)	STO D
4.	Key in gas flowrate W, lb/h	ENTER ↑
5.	Key in temperature T, °R	ENTER ↑
6.	Key in viscosity μ, lb/ft-h	ENTER ↑
7.	Key in length L, ft	A
8.	Key in molecular wt., M_w	ENTER ↑
9.	Key in gas compressibility factor Z	ENTER ↑
10.	Key in pipe diameter D, ft	R/S
11.	Key in P_1 and press the **C** key, (or P_2 and press the **B** key)	C or B
12.	Read the printout in the following order: M_1 (or M_2), N_{Re}, f, P_2 (or P_1), ΔP	
13.	Key in P_2 and press the **B** key, (or P_1 and press the **C** key)	B or C
14.	Read the printout for M_2 (or M_1), etc. (see step 12).	

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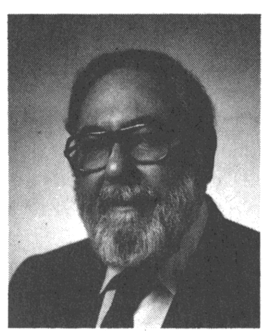
The author



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Calculating two-phase pressure drop

This program for the TI-59 calculator quickly determines pressure drop for two-phase fluids in horizontal lines.

W. Wayne Blackwell, *Ford, Bacon & Davis Texas, Inc.*

☐ A program having several novel features has been developed to determine two-phase pressure drop in horizontal lines. The program uses the semiempirical method of Lockhart and Martinelli [*3*], and is written for the Texas Instruments TI-59 programmable calculator used with the PC-100C printer, but will run without the printer.

The program:

- Calculates single-phase pressure drop in pipe for either gas or liquid flow.
- Calculates pressure drop in horizontal pipe for two-phase flow.
- Permits unusually rapid pressure-drop calculations—between 10 and 20 s for execution.
- Yields outputs adequate for permanent records.
- Permits easy change of operating data.
- Option-solves for ideal-gas density, using a self-prompting mode of operation.
- Can be used with a calculator without printer; pertinent calculated results are stored in data registers.

Considerable experimental and theoretical work has been carried out over the last 35 years on the prediction of two-phase frictional pressure drop in pipes.

Lockhart and Martinelli developed pressure-drop correlations in the late 1940s for water-air systems flowing in small pipes. These were later applied to other fluids in large lines.

The Lockhart-Martinelli correlations are most applicable to dispersed flow in which almost all the liquid is considered to be entrained as a spray in the gas phase. The correlations will yield slightly high results for stratified, wavy or slug flow. (These four regimes make up the bulk of two-phase flow configurations.) Annular flow is about the only flow regime for which the correlations may provide low results. (Annular flow is characterized by the liquid forming a film around the inside wall of the pipe, while the gas phase flows at high velocity as a central core.)

Thus, the Lockhart-Martinelli correlations will produce conservative results for the large majority of two-phase flow regimes. Since the time the equations were developed, other investigators have developed better ones for particular two-phase systems but, to this day, a better *general* correlation has not been worked out.

The basis of the Lockhart-Martinelli correlation is that the two-phase pressure drop is equal to the single-phase pressure drop of either phase, multiplied by a factor that is derived from the single-phase pressure drops of the two phases. In this program, the total pressure drop is based on the gas-phase ΔP by [*3*]:

$$\Delta P_{t(100)} = \Delta P_{g(100)} Y_g \quad (1)$$

The equations

The program solves the following equations*:

$$N_{Re} = 6.31 W_x/d\mu_x \quad (2)$$

$$f = 64/N_{Re} \quad \text{(for laminar or viscous flow, where } N_{Re} < 2{,}000) \quad (3)$$

$$f = (2 \log [(3.24\epsilon/d) + (7/N_{Re})^{0.9}])^{-2} \quad (4)$$

where $N_{Re} > 2{,}000$

$$\Delta P_{x(100)} = 0.000336(f)(W_x)^2/d^5\rho_x \quad (5)$$

$$X = [\Delta P_l/\Delta P_g]^{0.5} \quad (6)$$

$$Y_g = [\exp (A_0 + A_1 \ln X + A_2 \ln X^2 + A_3 \ln X^3)]^2 \quad (7)$$

$$V = 0.0509(W_g/\rho_g + W_l/\rho_l)/d^2$$

$$\rho_g = (M)(P)/10.73(T + 460)$$

Using the program

Table I presents the program operating instructions. The program is read in from a single magnetic card. To begin computations, the user must *first* press **B** to initialize the program, and *then* enter data for the gas and liquid phases in Registers R_1 to R_6. The user then keys in the pipe I.D. and presses **A** to obtain a complete printout of all pertinent information.

Pressure drop for single-phase flow is readily calcu-

*Eq. (2) and (5) are from Ref. 4; (4) is from Ref. 2; and (6) is from Ref. 1.

Originally published September 7, 1981.

Program for finding pressure drop in horizontal lines handling two-phase flow **Table I**

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
000	76	LBL	062	01	1	124	73	RC*	186	95	=	248	03	3
001	11	A	063	02	2	125	00	00	187	42	STO	249	42	STO
002	42	STO	064	01	1	126	65	×	188	18	18	250	00	00
003	15	15	065	69	OP	127	43	RCL	189	07	7	251	43	RCL
004	02	2	066	04	04	128	09	09	190	05	5	252	04	04
005	04	4	067	43	RCL	129	65	×	191	03	3	253	32	X:T
006	01	1	068	16	16	130	69	OP	192	03	3	254	00	0
007	06	6	069	69	OP	131	30	30	193	03	3	255	67	EQ
008	69	OP	070	06	06	132	69	OP	194	07	7	256	33	X^2
009	04	04	071	61	GTO	133	30	30	195	69	OP	257	61	GTO
010	43	RCL	072	24	CE	134	73	RC*	196	04	04	258	22	INV
011	15	15	073	76	LBL	135	00	00	197	43	RCL	259	76	LBL
012	69	OP	074	23	LNX	136	33	X^2	198	18	18	260	12	B
013	06	06	075	07	7	137	55	÷	199	69	OP	261	04	4
014	76	LBL	076	55	÷	138	43	RCL	200	06	06	262	08	8
015	22	INV	077	43	RCL	139	15	15	201	76	LBL	263	06	6
016	69	OP	078	14	14	140	45	Y^X	202	33	X^2	264	52	EE
017	20	20	079	95	=	141	05	5	203	43	RCL	265	94	+/-
018	73	RC*	080	45	Y^X	142	95	=	204	01	01	266	06	6
019	00	00	081	93	.	143	69	OP	205	55	÷	267	42	STO
020	65	×	082	09	9	144	06	06	206	43	RCL	268	08	08
021	43	RCL	083	95	=	145	97	DSZ	207	03	03	269	03	3
022	11	11	084	85	+	146	00	00	208	85	+	270	03	3
023	55	÷	085	53	(	147	25	CLR	209	43	RCL	271	06	6
024	43	RCL	086	43	RCL	148	61	GTO	210	04	04	272	52	EE
025	15	15	087	08	08	149	32	X:T	211	55	÷	273	94	+/-
026	55	÷	088	55	÷	150	76	LBL	212	43	RCL	274	06	6
027	69	OP	089	43	RCL	151	25	CLR	213	06	06	275	42	STO
028	20	20	090	15	15	152	55	÷	214	95	=	276	09	09
029	73	RC*	091	54	)	153	43	RCL	215	55	÷	277	93	.
030	00	00	092	95	=	154	13	13	216	43	RCL	278	00	0
031	95	=	093	28	LOG	155	95	=	217	15	15	279	05	5
032	42	STO	094	65	×	156	34	√X	218	33	X^2	280	00	0
033	14	14	095	02	2	157	42	STO	219	95	=	281	09	9
034	03	3	096	95	=	158	12	12	220	65	×	282	42	STO
035	05	5	097	33	X^2	159	04	4	221	43	RCL	283	10	10
036	01	1	098	35	1/X	160	04	4	222	10	10	284	06	6
037	07	7	099	42	STO	161	69	OP	223	95	=	285	93	.
038	69	OP	100	16	16	162	04	04	224	42	STO	286	03	3
039	04	04	101	02	2	163	43	RCL	225	19	19	287	01	1
040	43	RCL	102	01	1	164	12	12	226	04	4	288	42	STO
041	14	14	103	02	2	165	69	OP	227	02	2	289	11	11
042	69	OP	104	01	1	166	06	06	228	01	1	290	00	0
043	06	06	105	69	OP	167	71	SBR	229	07	7	291	42	STO
044	32	X:T	106	04	04	168	34	√X	230	02	2	292	00	00
045	02	2	107	43	RCL	169	76	LBL	231	07	7	293	42	STO
046	52	EE	108	16	16	170	35	1/X	232	69	OP	294	04	04
047	03	3	109	69	OP	171	42	STO	233	04	04	295	01	1
048	22	INV	110	06	06	172	17	17	234	43	RCL	296	42	STO
049	77	GE	111	76	LBL	173	04	4	235	19	19	297	06	06
050	23	LNX	112	24	CE	174	05	5	236	69	OP	298	01	1
051	06	6	113	07	7	175	02	2	237	06	06	299	93	.
052	04	4	114	05	5	176	02	2	238	00	0	300	04	4
053	55	÷	115	03	3	177	69	OP	239	42	STO	301	06	6
054	43	RCL	116	03	3	178	04	04	240	00	00	302	05	5
055	14	14	117	69	OP	179	43	RCL	241	98	ADV	303	09	9
056	95	=	118	04	04	180	17	17	242	25	CLR	304	42	STO
057	42	STO	119	43	RCL	181	69	OP	243	91	R/S	305	20	20
058	16	16	120	16	16	182	06	06	244	76	LBL	306	93	.
059	02	2	121	55	÷	183	65	×	245	32	X:T	307	04	4
060	07	7	122	69	OP	184	43	RCL	246	42	STO	308	09	9
061	02	2	123	20	20	185	13	13	247	13	13	309	01	1

(Continued) Table I

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
310	04	4	344	23	LNX	378	23	LNX	412	00	00	446	03	3
311	42	STO	345	65	×	379	33	X²	413	03	3	447	01	1
312	21	21	346	43	RCL	380	92	RTN	414	03	3	448	05	5
313	93	.	347	21	21	381	76	LBL	415	00	0	449	02	2
314	00	0	348	95	=	382	13	C	416	00	0	450	01	1
315	04	4	349	44	SUM	383	61	GTO	417	07	7	451	69	OP
316	08	8	350	24	24	384	35	1/X	418	01	1	452	04	04
317	09	9	351	43	RCL	385	76	LBL	419	69	OP	453	91	R/S
318	42	STO	352	12	12	386	14	D	420	03	03	454	42	STO
319	22	22	353	23	LNX	387	00	0	421	69	OP	455	27	27
320	03	3	354	33	X²	388	22	INV	422	05	05	456	99	PRT
321	93	.	355	65	×	389	90	LST	423	91	R/S	457	85	+
322	04	4	356	43	RCL	390	91	R/S	424	42	STO	458	04	4
323	08	8	357	22	22	391	76	LBL	425	26	26	459	06	6
324	07	7	358	95	=	392	15	E	426	99	PRT	460	00	0
325	94	+/-	359	44	SUM	393	69	OP	427	69	OP	461	95	=
326	52	EE	360	24	24	394	00	00	428	00	00	462	65	×
327	94	+/-	361	43	RCL	395	03	3	429	03	3	463	01	1
328	04	4	362	12	12	396	00	0	430	07	7	464	00	0
329	42	STO	363	23	LNX	397	04	4	431	06	6	465	93	.
330	23	23	364	33	X²	398	03	3	432	05	5	466	07	7
331	25	CLR	365	65	×	399	00	0	433	02	2	467	03	3
332	91	R/S	366	43	RCL	400	00	0	434	01	1	468	95	=
333	76	LBL	367	12	12	401	07	7	435	00	0	469	35	1/X
334	34	ΓX	368	23	LNX	402	01	1	436	00	0	470	65	×
335	00	0	369	65	×	403	69	OP	437	07	7	471	43	RCL
336	42	STO	370	43	RCL	404	03	03	438	01	1	472	25	25
337	24	24	371	23	23	405	69	OP	439	69	OP	473	65	×
338	43	RCL	372	95	=	406	05	05	440	03	03	474	43	RCL
339	20	20	373	44	SUM	407	91	R/S	441	69	OP	475	26	26
340	44	SUM	374	24	24	408	42	STO	442	05	05	476	95	=
341	24	24	375	43	RCL	409	25	25	443	05	5	477	69	OP
342	43	RCL	376	24	24	410	99	PRT	444	01	1	478	06	06
343	12	12	377	22	INV	411	69	OP	445	06	6	479	91	R/S

Fig. 2 Printouts for sample calculations

Abbreviations used in printout

- FF Friction factor, dimensionless
- ID Pipe internal dia., in.
- LFF Friction factor, laminar flow, dimensionless
- MW Molecular weight, dimensionless
- ΔP Pressure drop, psi
- ΔPT Pressure drop for two-phase flow, psi
- RE Reynolds number, dimensionless
- T Temperature, °F
- VEL Fluid velocity, ft/s
- X Lockhart-Martinelli 2-phase-flow modulus
- YG Y ordinate in Fig. 1 for turbulent/viscous flow
- */CF Density, lb/ft³

Two-phase flow

11.936	ID
18502848.53	RE
1.3073955-02	FF
1.1106016 00	ΔP
1.5859584 06	RE
1.3822176-02	FF
5.1501435-02	ΔP
2.1534288-01	X
5.2373116 00	YG
5.8165665 00	ΔPT
6.5722229 01	VEL
0.	00
350000.	01
0.01	02
2.	03
300000.	04
0.1	05
33.5	06

Single-phase flow

11.936	ID
18502848.53	RE
1.3073955-02	FF
1.1106016 00	ΔP
6.252277 01	VEL

Ideal density

MW ?	
18.	
P ?	
100.	
T°F ?	
300.	
.2207288959	*/CF

User instructions — **Table II**

Step	Procedure	Enter	Press	Display
1.	Load program	Side 1		1
		Side 2		2
2.	Initialize		**B**	0
3.	Enter required data*			
	W_g		**STO** 01	Data
	μ_g		**STO** 02	Data
	ρ_g		**STO** 03	Data
Two-phase only	W_l		**STO** 04	Data
	μ_l		**STO** 05	Data
	ρ_l		**STO** 06	Data
4.	Key in pipe I.D.			I.D.
5.	Calculate ΔP		**A**	Velocity

Options—For alternative pipe sizes, key in new pipe I.D. and press **A**
For alternative Y_g values, key in new Y_g and press **C**
For data printout, press **D**

*For single-phase pressure drop, enter either vapor or liquid data in Registers R_1 through R_3, and leave data Registers R_4 through R_6 as initialized (0 in R_4 and 1.0 in R_6).

User-defined keys — **Table III**

A. Starts program
B. Initializes program
C. Calculates ΔP with user Y_g
D. Lists data registers
E. Calculates ideal-gas density

described in the text

Turbulent flash viscous flow

```
     4.026      ID
109711.8728     RE
  1.994864-02   FF ---Turbulent flow (vapor)
 1.5525651-03   ΔP
 1.5673125 03   RE
 4.0834231-02   LFF ---Laminar (viscous) flow (liquid)
 3.8721307-06   ΔP
 4.9940179-02   X ---X value used in Fig. 1 for
 2.4195678 00   YG   finding YG
 3.7565364-03   ΔPT } These values automatically
 1.1084767 00   VEL   calculated for turbulent/turbulent
                      flow, but are ignored for this case.

       1.8      YG ---Y ordinate Fig. 1 for
.0027946171     ΔPT   turbulent/viscous flow
1.108476738     VEL   Pressure drop for
                      two-phase mixture
```

Data registers — **Table IV**

0.	Counter	14.	N_{Re}
1.	W_g or W_l, lb/h	15.	d, in.
2.	μ_g or μ_l, cP	16.	f
3.	ρ_g or ρ_l, lb/ft^3	17.	Y_g
4.	W_l or 0, lb/h	18.	$\Delta P_{t(100)}$, psi/100 ft
5.	μ_l, cP	19.	Velocity, ft/s
6.	ρ_l or 1.0, lb/ft^3	20.	A_0
7.	0	21.	A_1
8.	486 × 10^{-6}	22.	A_2
9.	336 × 10^{-6}	23.	A_3
10.	0.0509	24.	Sum register
11.	6.31	25.	M
12.	X	26.	P, psia
13.	$\Delta P_{g(100)}$, psi/100 ft	27.	T, °F

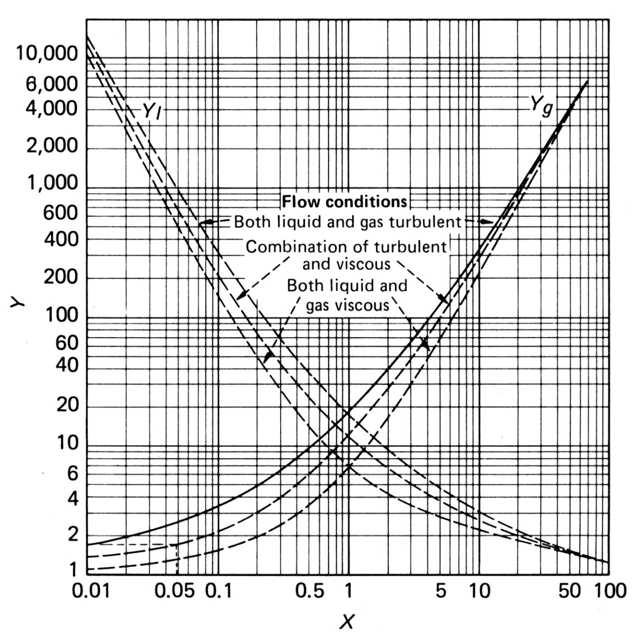
Registers 1 to 6 contain data stored by user. Remaining registers contain data stored, or calculated and stored, by program.

lated by storing the liquid or vapor data in Registers R_1 to R_3, keying in the pipe I.D., and pressing **A.** (When switching from two-phase flow to single-phase flow, the calculator must be reinitialized by pressing **B.**)

Two-phase flow

The program will calculate pressure drop for single-phase flow for either viscous or turbulent flow. However, for two-phase flow, it will calculate pressure drop only for turbulent flow.

Eq. (7) and constants A_0 through A_3 were obtained by a least-squares curve fit of the original data of Lockhart and Martinelli for the region in which both the liquid and gas flow are turbulent. This is the solid line in Fig. 1.



Parameters for pressure drop in liquid-gas flow through horizontal pipes [1] — **Fig. 1**

The other two curves of Fig. 1 represent either a combination of turbulent/viscous flow or viscous/viscous flow. Calculation of pressure involving these last two curves is so seldom encountered that it is not worthwhile to derive equations for each. However, by using Fig. 1, the user can determine an appropriate Y_g value and a correct pressure drop if a problem involves these two regimes.

The user need not bother with Fig. 1 for turbulent/turbulent flow, as the program will handle this automatically. For the other regimes, the user simply runs the program normally and then looks at the printed friction-factor value to see if laminar flow is encountered for either liquid or vapor. This is indicated by LFF in the program printout.

The X value calculated is located on Fig. 1, and a new Y_g (Y-axis) is read off for the type of flow encountered (turbulent/viscous, or viscous/viscous). This new value of Y_g is keyed into the machine, and the **C** key is pressed. The program calculates and prints a new value of $P_{t(100)}$ for these conditions (see Fig. 2).

The pipe roughness figure used in the program is 0.00015 ft (for steel pipe). Other values may be used by multiplying the roughness number by 3.24 and storing the result in Register 8. (Note that this must be done after the program is initialized by pressing Key **B.**)

To calculate ideal-gas density, the user must press **E** and answer the questions as they are presented. Press **R/S** after keying in each piece of data.

The user may press Key **D** at any time to obtain a printed listing of the data registers.

An example

What is the pressure drop per 100 ft of pipe in a 12-in., Schedule 40 line (I.D. = 11.936 in.), with the following flow data?

Vapor: W_g = 350,000 lb/h; μ_g = 0.01 cP; ρ_g = 2.0 lb/ft^3.

Liquid: W_l = 300,000 lb/h; μ_l = 0.10 cP; ρ_l = 33.5 lb/ft^3.

Assuming that the calculator has been initialized by Key **B,** the data are entered as follows:

R_1 = 350,000 (350,000, **STO,** 01); R_2 = 0.01; R_3 = 2.0; R_4 = 300,000; R_5 = 0.10; R_6 = 33.5. Then key in 11.936 (the pipe I.D.) and press Key **A.**

Turbulent/viscous flow example

What is the pressure drop per 100 ft of pipe having an I.D. of 4.026 in., with the following flow data?

Vapor: W_g = 700 lb/h; μ_g = 0.01 cP; ρ_g = 2.0 lb/ft^3.

Liquid: W_l = 100 lb/h; μ_l = 0.10 cP; ρ_l = 33.5 lb/ft^3.

Store data in R_1 to R_6 as in previous example. (Note: Press **B** first if this is the first run with program.) Key in 4.026 and press **A.**

After printout is complete, find Y_g from Fig. 1, using X calculated by program. Key in Y_g, and press Key **C.**

Nomenclature

A_0 to A_3	Constants for 2-phase-flow-modulus equation
d	Pipe I.D., in.
f	Friction factor, dimensionless
M	Molecular weight, dimensionless
N_{Re}	Reynolds number, dimensionless
$\Delta P_{g(100)}$	Pressure drop of gas flowing alone in pipe, psi/100 ft
$\Delta P_{l(100)}$	Pressure drop of liquid flowing alone in pipe, psi/100 ft
$\Delta P_{t(100)}$	Total pressure drop of 2-phase mixture, psi/100 ft
$\Delta P_{x(100)}$	Pressure drop of either liquid or gas as if flowing in pipe alone, psi/100 ft
T	Gas temperature, °F
V	Velocity of 2-phase mixture in pipe, ft/s
W_g	Gas flow, lb/h
W_l	Liquid flow, lb/h
W_x	Flow of gas or liquid, lb/h
X	Lockhart-Martinelli 2-phase-flow modulus
Y_g	Y ordinate in Fig. 1 (calculated by program itself for turbulent flow—for other types of flow, use Fig. 1)
ϵ	Pipe roughness, ft
μ_g	Gas viscosity, cP
μ_l	Liquid viscosity, cP
μ_x	Viscosity of liquid or gas, cP
ρ_g	Density of gas, lb/ft^3
ρ_l	Density of liquid, lb/ft^3
ρ_x	Density of liquid or gas, lb/ft^3

For HP-67/97 users

The HP version closely follows the TI program. The HP program listing appears in Table V, and the user instructions in Table VI. The HP printout corresponds to the TI output, but the HP has no "printed key." Please consult the table titled "Printouts for sample calculations described in the text" to identify the printout items for the HP output.

Program listing for HP version **Table V**

Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	012	1	01
002	STOA	35 11	013	×	-35
003	PRTX	-14	014	RCLA	36 11
004	*LBL3	21 03	015	÷	-24
005	2	02	016	RCL2	36 02
006	EEX	-23	017	÷	-24
007	3	03	018	PRTX	-14
008	RCL1	36 01	019	X>Y?	16-34
009	6	06	020	GTO1	22 01
010	.	-62	021	6	06
011	3	03	022	4	04

(Continued) Table V

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
023	X⇄Y	-41	047	X²	53	071	PRTX	-14	095	×	-35	119	RCLA	36 11
024	÷	-24	048	×	-35	072	RCLB	36 12	096	e^x	33	120	X²	53
025	GTO2	22 02	049	RCLA	36 11	073	÷	-24	097	PRTX	-14	121	÷	-24
026	*LBL1	21 01	050	5	05	074	√X	54	098	*LBLC	21 13	122	PRTX	-14
027	1/X	52	051	Y^x	31	075	PRTX	-14	099	RCLB	36 12	123	R/S	51
028	7	07	052	÷	-24	076	LN	32	100	×	-35	124	*LBLE	21 15
029	×	-35	053	RCL3	36 03	077	STOC	35 13	101	PRTX	-14	125	4	04
030	.	-62	054	÷	-24	078	RCL4	36 04	102	RCL1	36 01	126	6	06
031	9	09	055	F1?	16 23 01	079	RCL5	36 05	103	RCL3	36 03	127	0	00
032	Y^x	31	056	GTO2	22 02	080	RCLC	36 13	104	÷	-24	128	+	-55
033	RCL8	36 08	057	PRTX	-14	081	×	-35	105	STOD	35 14	129	1	01
034	RCLA	36 11	058	STOB	35 12	082	+	-55	106	*LBL1	21 01	130	0	00
035	÷	-24	059	RCL8	36 08	083	RCL6	36 06	107	.	-62	131	.	-62
036	+	-55	060	RCL9	36 09	084	RCLC	36 13	108	0	00	132	7	07
037	LOG	16 32	061	P⇄S	16-51	085	X²	53	109	5	05	133	3	03
038	2	02	062	STO9	35 09	086	×	-35	110	0	00	134	×	-35
039	×	-35	063	R↓	-31	087	+	-55	111	9	09	135	1/X	52
040	X²	53	064	STO8	35 08	088	RCL7	36 07	112	P⇄S	16-51	136	×	-35
041	1/X	52	065	RCL1	36 01	089	RCLC	36 13	113	RCL1	36 01	137	×	-35
042	*LBL2	21 02	066	X=0?	16-43	090	3	03	114	RCL3	36 03	138	PRTX	-14
043	PRTX	-14	067	GTO1	22 01	091	Y^x	31	115	÷	-24	139	RTN	24
044	RCL9	36 09	068	SF1	16 21 01	092	×	-35	116	RCLD	36 14	140	R/S	51
045	×	-35	069	GTO3	22 03	093	+	-55	117	+	-55			
046	RCL1	36 01	070	*LBL2	21 02	094	2	02	118	×	-35			

User instructions for HP version **Table VI**

1. Enter program, either manually or from magnetic card (two sides).
2. Store the following data:

	Primary Registers
Gas flow W_g, lb/h	**STO 1**
Gas viscosity, cP	**STO 2**
Gas density, lb/ft³	**STO 3**
Constant, 0.000486	**STO 8**
Constant, 0.000336	**STO 9**
Press **P ⇌ S**	Secondary Registers
Liquid flow W_l, lb/h	**STO 1**
Liquid viscosity, cP	**STO 2**
Liquid density, lb/ft³	**STO 3**
Constant, 1.4659	**STO 4**
Constant, 0.4914	**STO 5**
Constant, 0.0489	**STO 6**
Constant, -3.487E-4	**STO 7**
Press **P ↔ S** (Return to primary registers)	

3. Enter inside diameter, inches — Key **A**
4. Printout will be in same order as in original article.
5. If other than turbulent flow, select value of Y_g from Fig. 1, enter and press key **C**
6. For ideal gas density:
   - Enter molecular weight — **ENTER ↑**
   - Enter pressure, psia — **ENTER ↑**
   - Enter temperature, °F — Key **E**
   - Printout will be density, lb/ft³

References

1. Perry, Robert H., others, eds., "Chemical Engineers' Handbook," 4th ed., McGraw-Hill, New York, 1963.
2. Churchill, S. W., *AIChE J,* Vol. 19, No. 2, p. 375 (1973).
3. Lockhart, R. W., and Martinelli, R. C., *Chem Eng Prog,* pp. 39-48, Jan. 1949.
4. Crane Co., "Flow of Fluids Through Valves, Fittings and Pipe," Technical Paper No. 410, Crane Co., 300 Park Ave., New York, N.Y., 1976.

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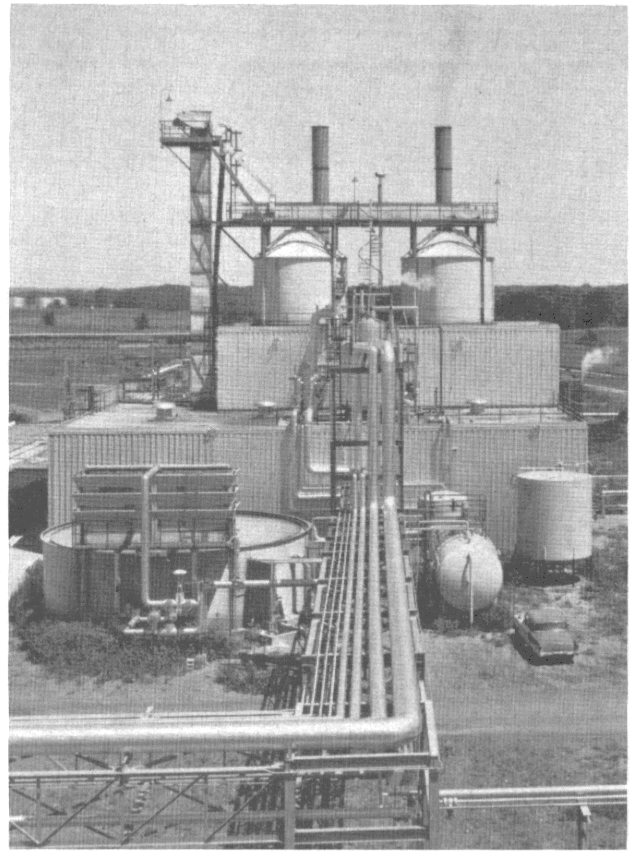
Program predicts pressure drop for steam flow

This TI-59 calculator program provides a fast, accurate estimate of pressure drop for saturated steam. Inlet pressure is the only physical datum required, because the program includes a routine that calculates specific volume.



Calvin R. Brunner, Malcolm Pirnie, Inc.

☐ Figuring the expected pressure drop in a saturated-steam line is a problem that comes up time and again in plant design and operations. When the length (or equivalent length) of the pipe is long, it is difficult to be accurate because the specific volume of the steam, and thus the velocity, changes along the way. This program, written for the TI-59 calculator with or without the PC-100C printer, eliminates the changing-density problem by dividing the pipe length into short increments over which the specific volume is assumed to be constant. The user controls the number of increments, and thus the run time and accuracy.

The calculation

The Unwin formula [*1*] expresses the pressure drop between two points as follows, assuming that there is no difference in height (gravity head):

$$P_1 - P_2 = 174.2 f w^2 \nu L / d^5 \quad (1)$$

where the friction factor f for turbulent flow of saturated steam is estimated by:

$$f = 0.0027(1 + 3.6/d) \quad (2)$$

The variables and units are defined in the nomenclature table. Combining Eq. 1 and 2, and converting

N = 10		*N* = 25		*N* = 100	
SATURATED STEAM FLOW		SATURATED STEAM FLOW		SATURATED STEAM FLOW	
3.826	DIA	3.826	DIA	3.826	DIA
7500.	LB/H	7500.	LB/H	7500.	LB/H
2000.	FEET	2000.	FEET	2000.	FEET
450.	P IN	450.	P IN	450.	P IN
10.	N	25.	N	100.	N
439.8921051	POUT	439.8843572	POUT	439.8808275	POUT

Printouts for example calculation show how accuracy increases with the number of iterations

Originally published February 22, 1982.

Specific-volume correlation for saturated steam — **Table I**

Pressure (P), psia	Specific volume (ν), ft^3/lb Actual	Calculated*
50	8.515	8.574
200	2.288	2.360
350	1.326	1.319
400	1.161	1.160
550	0.842	0.854

*Calculated as $\nu = 369.5\,P^{-0.962}$
Source of data: Ref. 2

Nomenclature

- d Pipe inside dia., in.
- f Friction factor
- L Total pipe length (or equivalent length), ft
- N Number of points for $N-1$ increments
- P Absolute pressure, psia
- s Incremental length $(=L/(N-1))$, ft
- w Steam flowrate, lb/s
- W Steam flowrate, lb/h
- ν Specific volume of steam, ft^3/lb

Program listing for TI-59 calculator — **Table II**

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
000	76	LBL	048	02	2	096	01	1	144	69	OP	192	07	7
001	11	A	049	07	7	097	94	+/-	145	03	03	193	69	OP
002	42	STO	050	05	5	098	44	SUM	146	02	2	194	04	04
003	00	00	051	05	5	099	06	06	147	01	1	195	43	RCL
004	91	R/S	052	04	4	100	43	RCL	148	02	2	196	03	03
005	76	LBL	053	05	5	101	07	07	149	07	7	197	69	OP
006	12	B	054	03	3	102	66	PAU	150	03	3	198	06	06
007	42	STO	055	05	5	103	97	DSZ	151	02	2	199	03	3
008	02	02	056	95	=	104	07	07	152	04	4	200	03	3
009	91	R/S	057	42	STO	105	00	00	153	03	3	201	00	0
010	76	LBL	058	01	01	106	63	63	154	69	OP	202	00	0
011	13	C	059	43	RCL	107	43	RCL	155	04	04	203	02	2
012	42	STO	060	05	05	108	06	06	156	69	OP	204	04	4
013	03	03	061	42	STO	109	98	ADV	157	05	05	205	03	3
014	91	R/S	062	06	06	110	03	3	158	98	ADV	206	01	1
015	76	LBL	063	43	RCL	111	06	6	159	01	1	207	69	OP
016	14	D	064	06	06	112	01	1	160	06	6	208	04	04
017	42	STO	065	45	Y^X	113	03	3	161	02	2	209	43	RCL
018	05	05	066	93	.	114	03	3	162	04	4	210	05	05
019	91	R/S	067	09	9	115	07	7	163	01	1	211	69	OP
020	76	LBL	068	06	6	116	04	4	164	03	3	212	06	06
021	15	E	069	02	2	117	01	1	165	69	OP	213	03	3
022	42	STO	070	94	+/-	118	03	3	166	04	04	214	01	1
023	04	04	071	95	=	119	05	5	167	43	RCL	215	69	OP
024	75	-	072	65	×	120	69	OP	168	00	00	216	04	04
025	01	1	073	03	3	121	01	01	169	69	OP	217	43	RCL
026	95	=	074	06	6	122	01	1	170	06	06	218	04	04
027	42	STO	075	09	9	123	03	3	171	02	2	219	69	OP
028	07	07	076	93	.	124	03	3	172	07	7	220	06	06
029	43	RCL	077	05	5	125	07	7	173	01	1	221	98	ADV
030	00	00	078	95	=	126	01	1	174	04	4	222	03	3
031	45	Y^X	079	42	STO	127	07	7	175	06	6	223	03	3
032	06	6	080	08	08	128	01	1	176	03	3	224	03	3
033	94	+/-	081	65	×	129	06	6	177	02	2	225	02	2
034	95	=	082	43	RCL	130	00	0	178	03	3	226	04	4
035	65	×	083	03	03	131	00	0	179	69	OP	227	01	1
036	03	3	084	65	×	132	69	OP	180	04	04	228	03	3
037	93	.	085	43	RCL	133	02	02	181	43	RCL	229	07	7
038	06	6	086	01	01	134	03	3	182	02	02	230	69	OP
039	85	+	087	65	×	135	06	6	183	69	OP	231	04	04
040	53	(	088	43	RCL	136	03	3	184	06	06	232	43	RCL
041	43	RCL	089	02	02	137	07	7	185	02	2	233	06	06
042	00	00	090	33	X²	138	01	1	186	01	1	234	69	OP
043	45	Y^X	091	55	÷	139	07	7	187	01	1	235	06	06
044	05	5	092	53	(	140	01	1	188	07	7	236	98	ADV
045	94	+/-	093	43	RCL	141	03	3	189	01	1	237	98	ADV
046	95	=	094	04	04	142	03	3	190	07	7	238	98	ADV
047	55	÷	095	75	-	143	00	0	191	03	3	239	91	R/S

User instructions **Table III**

Step	Keystrokes	Display
1. Partition	6 2nd Op 17	479.59
2. Enter program or read cards		
3. Enter data		
Diameter	*d* A	*d*
Flowrate	*W* B	*W*
Length	*L* C	*L*
Pressure in	P_1 D	P_1.
4. Enter no. of points	*N* E	Program runs. P_2 is final display. Results print out.
5. To change data, go back to Step 3.		
6. To change no. of points only, go back to Step 4.		

Storage locations **Table IV**

Register	Contents
00	Diameter (*d*)
01	Used
02	Flowrate (*W*)
03	Length (*L*)
04	No. of points (*N*)
05	Pressure in (P_1)
06	Pressure out (P_2)
07	Current increment
08	Specific volume (ν)
09	Pressure drop (P_1 - P_2)

flowrate to lb/h (W = 3,600 w), we obtain the general expression:

$$P_1 - P_2 = \frac{W^2 L\nu}{27{,}554{,}535}(d^{-5} + 3.6d^{-6}) \qquad (3)$$

The specific volume is a function of steam pressure, and varies with it as shown in Table I (for pressures to 550 psia):

$$\nu = 369.5\ P^{-0.962} \qquad (4)$$

If we now divide the pipe length (or equivalent length) L into $N - 1$ segments, each $s = L/(N - 1)$ in length, we can generalize Eq. 3 for the pressure drop across any segment:

$$P_i - P_j = \frac{W^2 s\nu_i}{27{,}554{,}535}(d^{-5} + 3.6d^{-6}) \qquad (5)$$

If s is sufficiently small, the pressure difference between points i and j is small enough that the difference between ν_i and ν_j is negligible.

The program calculates a new ν_i for each segment, and uses that value to calculate the pressure drop for the segment. This yields the pressure, and thus the ν_i value, for the next segment. The program is finished when it has gone through all $N - 1$ segments, and calculated the final pressure at length L. The greater the number of segments, the greater the accuracy of the result obtained.

How to use the program

Table II lists the program steps, and Table III the user instructions. Note that the calculator is partitioned to 479.59 when first turned on. Therefore, it is prepared for program entry or card reading (one card) automatically. While the program is running, a number will flash in the display, beginning at $N - 1$ and successively decreasing to 2. The last display is the final pressure P_2, and the results will print out as shown in the figure if the PC-100C printer is engaged.

The run time is about 2.5 s per iteration. For example, the calculation will take about 1 min if $N = 25$. To do a series of calculations, it is necessary to enter only the variable of interest and N. Entering N and pressing E starts the calculation procedure. If one wishes to retrieve any of the stored values without printing them out, the register locations are listed in Table IV.

Example: What is the pressure drop for 7,500 lb/h of 450-psia saturated steam flowing through 2,000 (equivalent) ft of 4-in. Sch. 40 pipe? (The inside diameter of such pipe is 3.826 in.) To solve the problem, enter the data as follows:

3.826 **A**
7,500 **B**
2,000 **C**
450 **D**

Then enter the number of increments desired, in this case 100:

The program runs for about 4.5 min, then prints out as shown in the figure on p. 112 (where N = 100). Note that the value for the final pressure is more accurate when N is greater. Since the final pressure shown is 439.8808275 psia, the pressure drop is 10 psi. One can also retrieve pressure drop directly from Register 09.

For HP-67/97 users

The HP version closely follows the TI program. Table V provides the HP program listing, and Table VI gives user instructions. A printout of the example results are contained in Table VII.

Program listing for HP version **Table V**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	020	3	03	039	RCL5	36 05	058	RCL1	36 01	077	PRTX	-14
002	STO0	35 00	021	.	-62	040	STO6	35 06	059	×	-35	078	RCL2	36 02
003	R/S	51	022	6	06	041	*LBLa	21 16 11	060	RCL4	36 04	079	DSP0	-63 00
004	*LBLB	21 12	023	×	-35	042	RCL6	36 06	061	÷	-24	080	PRTX	-14
005	STO2	35 02	024	RCL0	36 00	043	.	-62	062	RCL2	36 02	081	RCL3	36 03
006	R/S	51	025	5	05	044	9	09	063	X^2	53	082	PRTX	-14
007	*LBLC	21 13	026	CHS	-22	045	6	06	064	×	-35	083	RCL5	36 05
008	STO3	35 03	027	Y^x	31	046	2	02	065	STO9	35 09	084	PRTX	-14
009	R/S	51	028	+	-55	047	CHS	-22	066	CHS	-22	085	RCL4	36 04
010	*LBLD	21 14	029	2	02	048	Y^x	31	067	ST+6	35-55 06	086	PRTX	-14
011	STO5	35 05	030	7	07	049	3	03	068	RCLI	36 46	087	SPC	16-11
012	R/S	51	031	5	05	050	6	06	069	PSE	16 51	088	RCL6	36 06
013	*LBLE	21 15	032	5	05	051	9	09	070	DSZI	16 25 46	089	DSP9	-63 09
014	STO4	35 04	033	4	04	052	.	-62	071	GTOa	22 16 11	090	PRTX	-14
015	STOI	35 46	034	5	05	053	5	05	072	RCL6	36 06	091	SPC	16-11
016	RCL0	36 00	035	3	03	054	×	-35	073	DSP0	-63 00	092	SPC	16-11
017	6	06	036	5	05	055	STO8	35 08	074	SPC	16-11	093	SPC	16-11
018	CHS	-22	037	÷	-24	056	RCL3	36 03	075	RCL0	36 00	094	RTN	24
019	Y^x	31	038	STO1	35 01	057	×	-35	076	DSP3	-63 03	095	R/S	51

User instructions for HP version **Table VI**

Step	Procedure	Key	Display
1.	Key in program (or insert magnetic card, one side only)		
2.	Enter diameter *d*, in.	**A**	d
	Enter flow rate *W*, lb/h	**B**	W
	Enter length *L*, ft	**C**	L
	Enter inlet pressure P_1	**D**	P1
3.	Enter number of calculation steps *N* (Note: Increasing the number of steps from 25 to 100 would only increase pressure drop accuracy by about 0.03%; thus, there is no point in using more than 25 steps.) (Once the data are entered, to rerun for a different number of calculation steps, go directly to step 3.)	**E**	N

Output is: The calculation step number is intermittently displayed during the calculation. When *N* calculations have been made, the calculator prints:

Diameter, in.
Flow rate, lb/h
Length, ft
Inlet pressure, psia
Number of calculations
Outlet pressure, psia

Data are stored as follows:

Register	Data
0	Diameter
2	Flow rate
3	Length
4	Number of calculations
5	Inlet pressure
6	Outlet pressure
8	Specific volume, ft^3/lb
9	Pressure drop for the last calculation step

Note: Multiplying the value in Register 9 by the number of steps yields the total pressure drop, *approximately*.

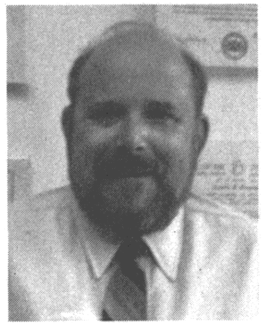
Printouts for example calculation-HP version **Table VII**

N = 10	3.826	***
	7500.	***
	2000.	***
	450.	***
	10.	***
	439.8908662	***
N = 25	3.826	***
	7500.	***
	2000.	***
	450.	***
	25.	***
	439.8841711	***
N = 100	3.826	***
	7500.	***
	2000.	***
	450.	***
	100.	***
	439.8886154	***

References

1. Baumeister, T., et al., eds., "Marks' Standard Handbook for Mechanical Engineers," 8th ed., McGraw-Hill Book Co., New York, 1978, p. 4-50.
2. Keenan, J. H., and Keyes, F. G., "Thermodynamic Properties of Steam," John Wiley & Sons, New York, 1936.

The author



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Estimate heat-tracing requirements for pipelines

Because the equations for tracing contain two unknown quantities, this calculator program contains a rapid procedure for determining the film heat-transfer coefficient to air. The program then continues to establish the remaining design values for heat tracing.

*W. Wayne Blackwell, Ford, Bacon & Davis, Texas Inc.**

☐ Pipelines containing liquids are often heat-traced to prevent the liquids from freezing or becoming too viscous to flow. Pipelines handling gases are sometimes heat-traced to prevent components or water vapor in the gases from condensing.

The program to be described will allow us to rapidly calculate the heat loss and tracing requirements for any given pipeline, using hot oil or other fluid medium as the heat source for the tracer. The program was written for the Texas Instruments TI-59 programmable calculator, to be used with the PC-100C printer.

This line-tracing program:

- Calculates surface temperature of insulated pipe.
- Calculates heat transferred per 100 ft of pipe.
- Calculates total heat transferred.
- Determines flowrate for hot media.
- Estimates number of heat tracers required without heat-transfer cement.
- Estimates number of heat tracers required with heat-transfer cement.

The program can be used without the printer because most results are stored in the TI-59 registers.

Equations for heat, flow and temperature

The program solves the following equations†:

$$Q = 2\pi K_i(T_a - T_s)/\ln(d_o/d_i) \tag{1}$$

$$Q = h_a(\pi d_o/12)(T_s - T_{air}) \tag{2}$$

$$X = \ln(d_o/d_i)(h_a)(d_o/12)/2K_i \tag{3}$$

$$T_s = (T_a + XT_{air})/(X + 1) \tag{4}$$

$$Q_t = QL_L \tag{5}$$

$$W = Q_t/C_p(T_{mi} - T_{mo}) \tag{6}$$

$$T_{woc} = Q/a(T_{med.avg.} - T_p) \tag{7}$$

$$T_{wc} = Q/b(T_{med.avg.} - T_p) \tag{8}$$

***To meet the author, see p. 111.**

†Eq. (1) and (2) are from Ref. 1; Eq. (7) and (8), Ref. 2; and Eq. (9), Ref. 3.

$$h_c + h_r = 564/(d_o)^{0.19}[273 - (T_s - T_{air})] \tag{9}$$

$$W_F = A + B(T_s - T_{air}) + C(T_s - T_{air})^2 \tag{10}$$

$$h_a = (h_c + h_r)W_F \tag{11}$$

Kern [*1*] and others have demonstrated that the heat transferred through an insulated pipe encounters four resistances: (1) film resistance on inside wall of pipe, (2) heat resistance through pipe wall, (3) heat resistance through insulation, and (4) air film resistance on outside of insulation. The first two resistances are normally very small, and have been neglected in this program.

For this program, Eq. (1) and (2) were equated, and the terms rearranged to form Eq. (4). Since Eq. (3) and (4) involve two unknowns (h_a and T_s), an initial value of h_a is assumed and T_s calculated. The program then calculates a new value of h_a from Eq. (9), and Eq. (4) is resolved for a new T_s. This procedure is repeated until the film heat-transfer coefficient changes less than 0.01 from the previous calculation.

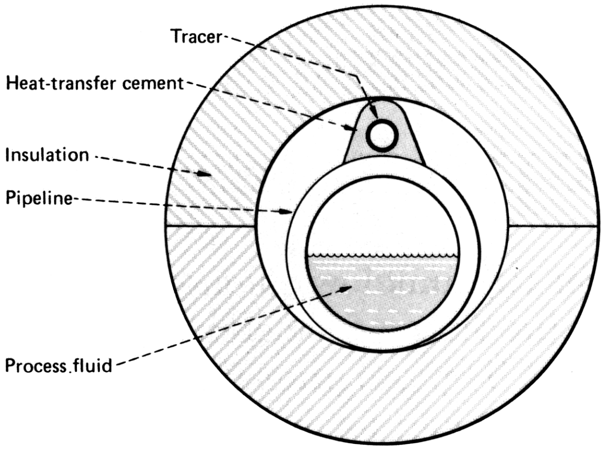
After T_s has been determined, the program continues to calculate Q, W, and the number of tracers, with and without transfer cement, required to maintain pipeline temperatures. Heat losses are based on a 20-mph wind speed, but may be adjusted for zero wind speed, as will shortly be explained.

Using the program

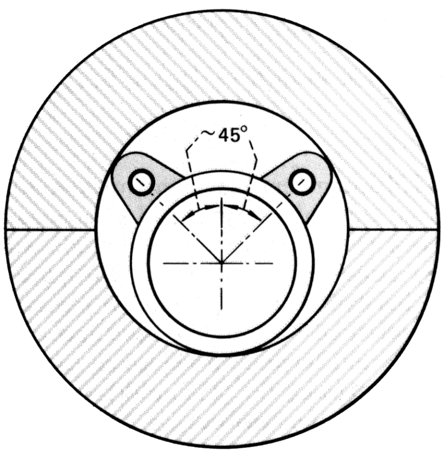
Table I lists the detailed program-operating instructions. After entry of the program (Steps 000 to 361) into program memory, and entry of the required constants in Storage Registers 18, 19, 20, 23, 24 and 25 (as outlined in Table III), the program and contents of the storage registers are down-loaded onto magnetic cards. Once this information has been thus stored, the program is ready for use.

The user need only read in the magnetic cards, store pertinent data in Storage Registers 0 through 10, and press **A** to begin the calculations (Table II). Usually a first guess of about 4 for h_a speeds up convergence and

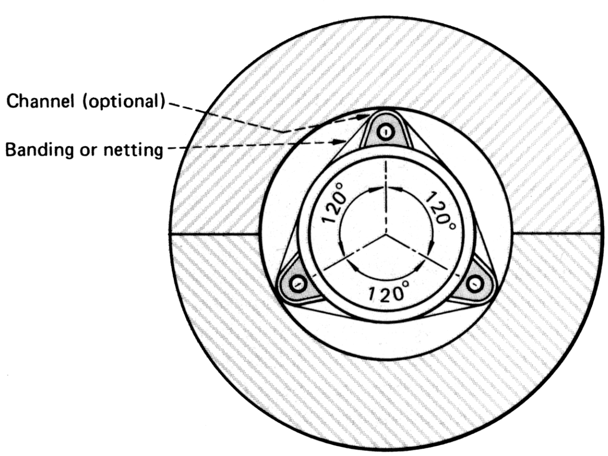
Originally published September 6, 1982.



Single tracer



Two tracers



Three tracers

Configuration for heat tracers depends on number required

Program for calculating total heat transferred, flowrate

Step	Code	Key
Start program		
000	76	LBL
001	11	A
002	69	OP
003	00	00
004	43	RCL
005	18	18
006	69	OP
007	01	01
008	43	RCL
009	19	19
010	69	OP
011	02	02
012	43	RCL
013	20	20
014	69	OP
015	03	03
016	69	OP
017	05	05
018	43	RCL
019	02	02
020	85	+
021	43	RCL
022	03	03
023	95	=
024	55	÷
025	02	2
026	95	=
027	42	STO
028	21	21
029	85	+
030	43	RCL
031	01	01
032	95	=
033	55	÷
034	02	2
035	95	=
036	42	STO
037	13	13
038	43	RCL
039	05	05
040	85	+
041	43	RCL
042	06	06
043	95	=
044	42	STO
045	12	12
046	85	+
047	53	(
048	43	RCL
049	07	07
050	65	×
051	02	2
052	54	)
053	95	=
054	42	STO
055	11	11
056	76	LBL
057	12	B
Calculate T_s		
058	43	RCL
059	11	11
060	55	÷
061	43	RCL
062	12	12
063	95	=
064	23	LNX
065	65	×
066	43	RCL
067	10	10
068	65	×
069	43	RCL
070	11	11
071	55	÷
072	01	1
073	02	2
074	55	÷
075	02	2
076	55	÷
077	43	RCL
078	08	08
079	95	=
080	42	STO
081	16	16
082	65	×
083	43	RCL
084	04	04
085	85	+
086	43	RCL
087	13	13
088	95	=
089	55	÷
090	53	(
091	43	RCL
092	16	16
093	85	+
094	01	1
095	54	)
096	95	=
097	42	STO
098	14	14
099	76	LBL
100	13	C
Calculate $h_c + h_r$		
101	43	RCL
102	11	11
103	45	Y^X
104	93	.
105	01	1
106	09	9
107	95	=
108	65	×
109	53	(
110	02	2
111	07	7
112	03	3
113	75	-
114	53	(
115	43	RCL
116	14	14
117	75	-
118	43	RCL
119	04	04
120	54	)
121	95	=
122	35	1/X
123	65	×
124	05	5
125	06	6
126	04	4
127	95	=
128	42	STO
129	22	22
130	43	RCL
131	14	14
132	75	-
133	43	RCL
134	04	04
135	95	=
136	42	STO
137	27	27
138	43	RCL
Calculate wind factor		
139	23	23
140	42	STO
141	26	26
142	43	RCL
143	27	27
144	65	×
145	43	RCL
146	24	24
147	95	=
148	44	SUM
149	26	26
150	43	RCL
151	27	27
152	33	X^2
153	65	×
154	43	RCL
155	25	25
156	95	=
157	44	SUM
158	26	26
159	43	RCL
160	26	26
161	65	×
162	43	RCL
163	22	22
164	95	=
Calculate h_a		
165	42	STO
166	28	28
167	93	.
168	00	0
169	01	1
170	32	X:T
171	43	RCL
172	10	10
173	75	-
174	43	RCL
175	28	28
176	95	=
177	50	I×I

of heat-transfer medium, and number of heat tracers **Table I**

Step	Code	Key
178	77	GE
179	15	E
180	76	LBL
181	14	D
Calculate variables		
182	69	OP
183	00	00
184	03	3
185	07	7
186	03	3
187	06	6
188	69	OP
189	04	04
190	43	RCL
191	14	14
192	69	OP
193	06	06
194	43	RCL
195	28	28
196	65	×
197	89	π
198	65	×
199	43	RCL
200	11	11
201	55	÷
202	01	1
203	02	2
204	65	×
205	53	(
206	43	RCL
207	14	14

Step	Code	Key
208	75	-
209	43	RCL
210	04	04
211	54	)
212	95	=
213	42	STO
214	15	15
215	69	OP
216	00	00
217	03	3
218	04	4
219	69	OP
220	04	04
221	43	RCL
222	15	15
223	69	OP
224	06	06
225	01	1
226	04	4
227	03	3
228	07	7
229	04	4
230	01	1
231	02	2
232	03	3
233	69	OP
234	04	04
235	43	RCL
236	15	15
237	65	×
238	43	RCL
239	00	00
240	95	=
241	69	OP

Step	Code	Key
242	06	06
243	55	÷
244	43	RCL
245	09	09
246	55	÷
247	53	(
248	43	RCL
249	02	02
250	75	-
251	43	RCL
252	03	03
253	54	)
254	95	=
255	42	STO
256	17	17
257	02	2
258	07	7
259	01	1
260	04	4
261	06	6
262	03	3
263	02	2
264	03	3
265	69	OP
266	04	04
267	43	RCL
268	17	17
269	69	OP
270	06	06
271	43	RCL
272	21	21
273	75	-
274	43	RCL
275	01	01

Step	Code	Key
276	95	=
277	42	STO
278	29	29
279	65	×
Constant *a*		
280	93	.
281	03	3
282	09	9
283	03	3
284	95	=
285	35	1/X
286	65	×
287	43	RCL
288	15	15
289	95	=
290	85	+
291	93	.
292	09	9
293	09	9
294	09	9
295	95	=
296	59	INT
297	32	X:T
298	03	3
299	07	7
300	04	4
301	03	3
302	03	3
303	02	2
304	01	1
305	05	5

Step	Code	Key
306	69	OP
307	04	04
308	32	X:T
309	69	OP
Print T_{woc}		
310	06	06
311	43	RCL
312	29	29
313	65	×
Constant *b*		
314	04	4
315	93	.
316	05	5
317	08	8
318	95	=
319	35	1/X
320	65	×
321	43	RCL
322	15	15
323	95	=
324	85	+
325	93	.
326	09	9
327	09	9
328	09	9
329	95	=
330	59	INT
331	32	X:T
332	69	OP
333	00	00
334	03	3
335	07	7

Step	Code	Key
336	04	4
337	03	3
338	01	1
339	05	5
340	69	OP
341	04	04
342	32	X:T
343	69	OP
Print T_{wc}		
344	06	06
345	98	ADV
346	91	R/S
347	76	LBL
348	15	E
Readjust h_a		
349	43	RCL
350	28	28
351	42	STO
352	10	10
353	61	GTO
354	12	B
355	91	R/S
356	76	LBL
357	10	E'
Print data registers		
358	00	0
359	22	INV
360	90	LST
361	91	R/S
End program		

reduces run time. After a program run, intermediate results are maintained in unused Storage Registers 11 through 29. See Table III for all stored information.

In this program, the combined convection and radiation heat-transfer coefficients are corrected by a wind factor to calculate h_a. If designing for zero wind conditions, enter 1.0 in Storage Register 23, 0 in Storage Registers 24 and 25, and run the program as usual.

Thermal conductance values, *a* and *b*, used in this program are for ½-in. tracer lines. The user may substi-

Nomenclature

A,B,C	Constants for wind-factor equation
a	Thermal conductance, tracer to pipe, without heat-transfer cement, Btu/(h)(°F)(ft of pipe)
b	Thermal conductance, tracer to pipe, with cement, Btu/(h)(°F)(ft of pipe)
C_p	Specific heat of hot medium, Btu/(lb)(°F)
d_i	Inside diameter of insulation, in.
d_o	Outside diameter of insulation, in.
h_a	Film heat-transfer coefficient to air (corrected for wind), Btu/(h)(°F)(ft²)
$h_c + h_r$	Combined convection and radiation heat-transfer coefficient, Btu/(h)(°F)(ft²)
K_i	Thermal conductivity of insulation, Btu/(h)(ft²)(°F/ft)
L_L	Total pipeline length, ft
Q	Heat lost per ft of pipe, Btu/(h)(ft)
Q_t	Total heat lost from pipeline, Btu/h
T_a	Average temperature of pipe and tracer, °F
T_{air}	Air temperature, °F
$T_{med.avg.}$	Average temperature of hot medium, °F
T_{mi}	Inlet temperature of hot medium, °F
T_{mo}	Outlet temperature of hot medium, °F
T_p	Temperature in pipe, °F
T_s	Outside surface temperature of insulation, °F
T_{wc}	Number of tracers required with heat-transfer cement
T_{woc}	Number of tracers required without heat-transfer cement
W	Flowrate of hot medium, lb/h
W_F	Wind factor

User instructions — **Table II**

Step	Procedure	Enter	Press	Display
1.	Read in both magnetic cards, Sides 1, 2 and 4		CLR	1, 2, 4
2.	Store data in registers R0 through R10	R0 = L_L		
		R1 = T_p		Data
		R2 = T_{mi}		
		R3 = T_{mo}		
		R4 = T_{air}		
		R5 = Pipe O.D.		
		R6 = Tracer allowance		
		R7 = T_k		
		R8 = K_i		
		R9 = C_p		
		R10 = h_a (est.)		
3.	Press A to begin computations		A	T_{wc}
4.	Option: Press E' for printout of data registers		E'	0

Contents of data registers — **Table III**

0. Line length, ft	15. Q, Btu/(h)(ft)
1. T_p, °F	16. X
2. T_{mi}, °F	17. W, lb/h
3. T_{mo}, °F	18. 2724311700*
4. T_{air}, °F	19. 3735131517*
5. Pipe O.D., in.	20. 3500332230*
6. Tracer allowance, in.	21. $T_{med. avg.}$, °F
7. T_k, in.	22. $h_c + h_r$, Btu/(h)(°F)(ft²)
8. K_i, Btu/(h)(ft²)(°F/ft)	23. 2.814*
9. C_p, Btu/(lb)(°F)	24. −0.0003885714*
10. h_a (trial calculation, Btu/(h)(°F)(ft²)	25. −0.0000012857*
11. d_o, in.	26. W_F
12. d_i, in.	27. $T_s - T_{air}$, °F
13. $T_{avg. inside}$, °F	28. h'_a, Btu/(h)(°F)(ft²)
14. T_s, °F	29. $T_{med. avg.} - T_p$, °F

*Constants that must be stored on magnetic card before program execution (first time only).

tute constants for other-sized tracers, as given in Table IV. Constant a occupies Program Steps 280 through 283, and b occupies Steps 314 through 317. Constants for other-sized tracer lines may be keyed into the same area of the program.

An example

Estimate the number of tracers required to maintain 100 ft of 6-in.-dia. process line at 500°F. Hot tracing medium is available at 625°F, and has a heat capacity of 0.53 Btu/(lb)(°F). The process line is covered with 2.5 in. of insulation whose thermal conductivity is 0.037 Btu/(h)(ft²)(°F/ft). Design this system for 0°F air temperature and 20-mph winds. The tracing medium is to be returned at 550°F. Use ½-in. tracers.

Thermal conductance values for tracer lines — **Table IV**

Tube size, in.	Constant, a	Constant, b
3/8	0.295	3.44
1/2	0.393	4.58
5/8	0.490	5.73

See Eq. (7) and (8)

User-defined keys — **Table V**

- **A** – Starts program
- **B** – Calculates T_s (internal)
- **C** – Calculates $h_c + h_r$ (internal)
- **D** – Calculates Q, Q_t, W, and number of tracers (internal)
- **E** – Readjusts h_a for new trial (internal)
- **E'** – Prints data registers

Enter the problem variables into the calculator:

Variable	Register	Variable	Register
$L_L = 100$	(R0)	Tracer	
$T_p = 500$	(R1)	allowance* = 1.25	(R6)
$T_{mi} = 625$	(R2)	$T_k = 2.5$	(R7)
$T_{mo} = 550$	(R3)	$K_i = 0.037$	(R8)
$T_{air} = 0$	(R4)	$C_p = 0.53$	(R9)
Pipe O.D. = 6.065	(R5)	h_a (trial) = 4.0	(R10)

Press Key **A** to run the program. The results print as:

```
LINE TRACER PGM
 18.84804484      TS
 234.8519058       Q
 23485.19058    BTUH
 590.8224045    LB/H
          7.    TWOC
          1.     TWC
```

The estimated number of tracers without the heat-transfer cement for this example is seven, while using a heat-transfer cement reduces the required number to one. Circulation rate of the tracing medium is 590.8 lb/h, and heat lost from 100 ft of pipeline is 23,485 Btu/h.

Users not having a printer may recall most of the calculated results from the data registers (see Table III). The value displayed after program execution is T_{wc}.

For HP-67/97 users

The HP version closely follows the TI program. Table VI offers the HP program listing, and Table VII provides user instructions for the HP version. Table VIII lists the contents of the HP data registers.

*Allow approximately 1¼ in. between the pipe and insulation to accommodate the ½-in. tracer line and heat-transfer cement. For three, or more, tracers, allow twice this value. Smaller tracers may require only ⅞ to 1 in. of space. Tracers are normally spaced equidistant around the pipe (see illustration), and are run parallel to the pipe. A final run with the calculator program may be made after the total number of tracers and spacing has been established.

Program listing for HP version **Table VI**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	040	2	02	079	STOE	35 15	118	2	02	157	9	09
002	P⇄S	16-51	041	÷	-24	080	RCL4	36 04	119	÷	-24	158	5	05
003	RCL2	36 02	042	2	02	081	P⇄S	16-51	120	RCL4	36 04	159	+	-55
004	RCL3	36 03	043	÷	-24	082	RCL4	36 04	121	P⇄S	16-51	160	INT	16 34
005	+	-55	044	P⇄S	16-51	083	-	-45	122	RCL4	36 04	161	DSP0	-63 00
006	2	02	045	RCL8	36 08	084	STOB	35 12	123	-	-45	162	PRTX	-14
007	÷	-24	046	÷	-24	085	P⇄S	16-51	124	×	-35	163	RCLB	36 12
008	P⇄S	16-51	047	STOD	35 14	086	RCL7	36 07	125	P⇄S	16-51	164	4	04
009	STO6	35 06	048	RCL4	36 04	087	STO0	35 00	126	STO5	35 05	165	.	-62
010	P⇄S	16-51	049	×	-35	088	RCLB	36 12	127	PRTX	-14	166	5	05
011	RCL1	36 01	050	P⇄S	16-51	089	RCL8	36 08	128	P⇄S	16-51	167	8	08
012	+	-55	051	RCL3	36 03	090	×	-35	129	RCL0	36 00	168	×	-35
013	2	02	052	+	-55	091	ST+0	35-55 00	130	×	-35	169	1/X	52
014	÷	-24	053	RCLD	36 14	092	RCLE	36 15	131	PRTX	-14	170	RCL5	36 05
015	P⇄S	16-51	054	1	01	093	X²	53	132	RCL9	36 09	171	×	-35
016	STO3	35 03	055	+	-55	094	RCL9	36 09	133	÷	-24	172	.	-62
017	P⇄S	16-51	056	÷	-24	095	×	-35	134	RCL2	36 02	173	9	09
018	RCL5	36 05	057	STO4	35 04	096	ST+0	35-55 00	135	RCL3	36 03	174	9	09
019	RCL6	36 06	058	*LBLC	21 13	097	RCL0	36 00	136	-	-45	175	9	09
020	+	-55	059	RCL1	36 01	098	RCLE	36 15	137	÷	-24	176	+	-55
021	P⇄S	16-51	060	.	-62	099	×	-35	138	PRTX	-14	177	INT	16 34
022	STO2	35 02	061	1	01	100	STOC	35 13	139	STOI	35 46	178	PRTX	-14
023	P⇄S	16-51	062	9	09	101	RCLA	36 11	140	P⇄S	16-51	179	DSP2	-63 02
024	RCL7	36 07	063	Y^X	31	102	-	-45	141	RCL6	36 06	180	R/S	51
025	2	02	064	2	02	103	ABS	16 31	142	P⇄S	16-51	181	*LBLE	21 15
026	×	-35	065	7	07	104	.	-62	143	RCL1	36 01	182	RCLC	36 13
027	+	-55	066	3	03	105	0	00	144	-	-45	183	STOA	35 11
028	P⇄S	16-51	067	RCL4	36 04	106	1	01	145	STOB	35 12	184	GTOB	22 12
029	STO1	35 01	068	P⇄S	16-51	107	X≤Y?	16-35	146	.	-62	185	R/S	51
030	*LBLB	21 12	069	RCL4	36 04	108	GTOE	22 15	147	3	03	186	*LBLe	21 16 15
031	RCL1	36 01	070	-	-45	109	*LBLD	21 14	148	9	09	187	DSP9	-63 09
032	RCL2	36 02	071	-	-45	110	RCL4	36 04	149	3	03	188	PREG	16-13
033	÷	-24	072	×	-35	111	PRTX	-14	150	×	-35	189	DSP2	-63 02
034	LN	32	073	1/X	52	112	RCLC	36 13	151	1/X	52	190	RTN	24
035	RCLA	36 11	074	5	05	113	Pi	16-24	152	P⇄S	16-51	191	R/S	51
036	×	-35	075	6	06	114	×	-35	153	RCL5	36 05			
037	RCL1	36 01	076	4	04	115	RCL1	36 01	154	×	-35			
038	×	-35	077	×	-35	116	×	-35	155	.	-62			
039	1	01	078	P⇄S	16-51	117	1	01	156	9	09			

User instructions for HP version **Table VII**

Store the following data:		
Pipeline length, ft	L_L	**STO 0**
Temperature in pipe, °F	T_p	**STO 1**
Inlet temperature, hot medium, °F	T_{mi}	**STO 2**
Outlet temperature, hot medium, °F	T_{mo}	**STO 3**
Air temperature, °F	T_{air}	**STO 4**
Pipe OD, in.		**STO 5**
Tracer allowance, in.		**STO 6**
Insulation thickness, in.	T_k	**STO 7**
Thermal conductivity of insulation, Btu/(h)(ft²)(°F/ft)	K_i	**STO 8**
Heat capacity of hot medium, Btu/(lb)(°F)	C_p	**STO 9**
Air film coefficient, estimate, Btu/(h)(°F)(ft²)	h_a	**STO A**
Exchange registers		**P ⇄ S**
Store constants:	2.814	**STO 7**
(See note below)	–3.885712E–4	**STO 8**
	–1.285E–6	**STO 9**

Run program with key **A**

(Continued) Table VII

Printed output is:

Surface temperature of insulation, °F	T_s
Heat loss per foot of pipe, Btu/h	Q
Total heat loss, Btu/h	Q_t
Flow rate of hot medium, lb/h	W
Number of tracers required:	
without transfer cement	T_{woc}
with transfer cement	T_{wc}

Note: When designing for zero wind conditions, enter the following constants in the place of those given above, 1.0, 0 and 0 in secondary registers 7, 8 and 9.

Contents of data registers—HP version Table VIII

HP	TI		HP	TI	
0	26	W_F	D	16	X
1	11	d_o, in.	E	22	$h_c + h_r$, Btu/(h)(°F)(ft^2)
2	12	d_i, in.	S0	0	line length, ft
3	13	$T_{avg\ inside}$, °F	S1	1	T_p, °F
4	14	T_s, °F	S2	2	T_{mi}, °F
5	15	Q, Btu/(h)(ft)	S3	3	T_{mo}, °F
6	21	$T_{med,\ avg}$, °F	S4	4	T_{air}, °F
7	23	2.814	S5	5	pipe O.D., in.
8	24	-0.0003885714	S6	6	tracer allowance, in.
9	25	-0.0000012857	S7	7	T_k, in.
A	10	h_a (trial calculation, Btu/(h)(°F)(ft^2))	S8	8	K_i, Btu/(h)(ft^2)(°F/ft)
B	29	$T_{med,\ avg} - T_p$, °F	S9	9	C_p, Btu/(lb)(°F)
C	28	h'_a, Btu/(h)(°F)(ft^2)			

References

1. Kern, D. Q., "Process Heat Transfer," pp. 18–20, McGraw-Hill, New York, 1950.
2. Kohli, I. P., *Chem. Eng.*, Mar. 26, 1979, p. 163.
3. Kuong, J. F., *Chem. Eng.*, July 25, 1960, p. 146.

Estimate equivalent line lengths of piping circuits

Quickly determine the equivalent line lengths of loops containing fittings, valves, and pipes of various lengths. All that is needed is an isometric drawing of the piping system, and this program for the TI-59 calculator.

*W. Wayne Blackwell, Ford, Bacon & Davis, Inc.**

☐ The program calculates equivalent pipe lengths for eight types of valves, eight types of fittings, and entrance and exit losses. It then sums the equivalent pipe lengths and prints the total. Next, it adds pipe lengths in feet and inches (tedious ft/in. conversions are not necessary), and prints the total equivalent feet in decimal form. With this information, the total pressure drop through a circuit can be readily determined.

Each valve, fitting and loss is identified, and the number of each is listed, in the printout. The program prompts the user for part of the input.

Although written for the TI-59 calculator and the PC-100C printer, the program could be used without a printer, because all totals are stored in data registers.

Program development

The pressure drop through valves and fittings is related to velocity changes in the flowing fluid:

$$h = KV^2/2g$$

Here, h = pressure loss in head of fluid, ft; K = experimental coefficient (number of velocity heads); V = average velocity in pipe, ft/s; and g = 32.17 ft/s^2.

Pressure drops calculated via the foregoing equation (which is for turbulent flow) usually give accurate pressure losses for valves and fittings. However, velocity and K data are required to solve the equation.

The equivalent-length method, though less accurate,

*For information about the author, see *Chem. Eng.*, July 12, p. 108.

Originally published November 1, 1982.

User instructions and key definitions for calculating equivalent line lengths — Table I

Step	Procedure	Enter	Press	Display
1.	Partition calculator at 719.29	3	2nd OP 17	719.29
2.	Read in both sides of two magnetic cards	CLR		1,2,3,4
3.	Press A to begin computation		A	*Print*
4.	When calculator stops, key in pipe I.D. and press R/S		R/S	0
5.	Press subroutine label corresponding to type of valve, fitting or loss		Lbl, SBR*	*Print*
6.	Key in number of valves or fittings and press R/S		R/S	0
7.	Repeat Steps 5 and 6 until equivalent lengths of all valves and fittings have been calculated		Lbl, SBR*	*Print*
8.	Press C′ for sum of equivalent length of pipe		C′	0
9.	Press E′ to activate sum of pipe-length program		E′	*Print*
10.	Enter pipe length as feet; for example 8 ft, 10½ in. as 8.105			*Length*
11.	Press R/S			*in/ft*
12.	After calculation has stopped, repeat Steps 10 and 11 until all pipe lengths have been entered			0
13.	Press C′ for sum of pipe lengths		C′	0

*To activate user labels A through E (or A′ through E′), press only the appropriate key. To call other labels, press SBR, then the label; (for example, Label X^2 is called by SBR X^2.

User-defined keys

A	Starts program	CLR	Ball check valves
B	Gate valves	x⇌t	Butterfly valves
C	Long-radius 90-deg. elbows	X^2	Three-way straight-through valves
D	Straight-through tees	√X	Three-way flow-through branch valves
E	Reduction/enlargement	1/X	Short-radius 90-deg. elbows
A′	Entrance loss	STO	Short-radius 45-deg. elbows
B′	Exit loss	RCL	90-deg. miter bends
C′	Sum of equivalent feet	SUM	45-deg. miter bends
INV	Globe valves	Y^x	Flow-through branch tees
ln x	Plug valves	E′	Activates sum-of-pipe-length program
CE	Swing check valves		

Sample problem yields equivalent length of 135 ft — Table II

```
EQUIVALENT LINE                    LINE LNGTH
LENGTH PROGRAM                           2.04
PIPE ID ?                              10.115
         4.026         IN                  7.
LR90 ELBOWS ?                          5.0325
            3.                     SUM-EQL FT
     20.17026          FT             25.5625
BF TEES ?
            1.
        20.13          FT
GATE VALVES ?
            1.
       4.4286          FT
SWCK VALVES ?
            1.
      44.04444         FT
EXIT
   20.56124573         FT
SUM-EQL FT
   109.3345457
```

Program calculates equivalent line lengths for piping loops containing valves, fittings, and piping of various lengths

Step	Code	Key
000	76	LBL
001	99	PRT
002	65	×
003	43	RCL
004	07	07
005	95	=
006	44	SUM
007	00	00
008	42	STO
009	19	19
010	43	RCL
011	22	22
012	69	OP
013	04	04
014	43	RCL
015	19	19
016	69	OP
017	06	06
018	00	0
019	69	OP
020	04	04
021	91	R/S

Pipe I.D.

Step	Code	Key
022	76	LBL
023	11	A
024	69	OP
025	00	00
026	43	RCL
027	01	01
028	69	OP
029	01	01
030	43	RCL
031	02	02
032	69	OP
033	02	02
034	43	RCL
035	03	03
036	69	OP
037	03	03
038	69	OP
039	05	05
040	43	RCL
041	04	04
042	69	OP
043	01	01
044	43	RCL
045	05	05
046	69	OP
047	02	02
048	43	RCL
049	06	06
050	69	OP
051	03	03
052	69	OP
053	05	05
054	69	OP
055	00	00
056	03	3
057	03	3
058	02	2
059	04	4
060	03	3
061	03	3
062	01	1
063	07	7
064	00	0
065	00	0
066	69	OP
067	01	01
068	02	2
069	04	4
070	01	1
071	06	6
072	00	0
073	00	0
074	07	7
075	01	1
076	00	0
077	00	0
078	69	OP
079	02	02
080	69	OP
081	05	05
082	02	2
083	04	4
084	03	3
085	01	1
086	69	OP
087	04	04
088	91	R/S
089	42	STO
090	07	07
091	69	OP
092	06	06
093	00	0
094	42	STO
095	00	00
096	69	OP
097	04	04
098	91	R/S

Gate valves

Step	Code	Key
099	76	LBL
100	12	B
101	02	2
102	02	2
103	01	1
104	03	3
105	03	3
106	07	7
107	01	1
108	07	7
109	00	0
110	00	0
111	69	OP
112	01	01
113	71	SBR
114	52	EE
115	91	R/S
116	99	PRT
117	65	×
118	01	1
119	93	.
120	01	1
121	00	0
122	61	GTO
123	99	PRT

Valves

Step	Code	Key
124	76	LBL
125	52	EE
126	43	RCL
127	20	20
128	69	OP
129	02	02
130	43	RCL
131	21	21
132	69	OP
133	03	03
134	69	OP
135	05	05
136	92	RTN

Globe valves

Step	Code	Key
137	76	LBL
138	22	INV
139	02	2
140	02	2
141	02	2
142	07	7
143	01	1
144	04	4
145	01	1
146	07	7
147	00	0
148	00	0
149	69	OP
150	01	01
151	71	SBR
152	52	EE
153	91	R/S
154	99	PRT
155	65	×
156	02	2
157	08	8
158	93	.
159	03	3
160	03	3
161	61	GTO
162	99	PRT

Plug valves

Step	Code	Key
163	76	LBL
164	23	LNX
165	03	3
166	03	3
167	02	2
168	07	7
169	04	4
170	01	1
171	02	2
172	02	2
173	00	0
174	00	0
175	69	OP
176	01	01
177	71	SBR
178	52	EE
179	91	R/S
180	99	PRT
181	65	×
182	01	1
183	93	.
184	05	5
185	61	GTO
186	99	PRT

Swing check valves

Step	Code	Key
187	76	LBL
188	24	CE
189	03	3
190	06	6
191	04	4
192	03	3
193	01	1
194	05	5
195	02	2
196	06	6
197	00	0
198	00	0
199	69	OP
200	01	01
201	71	SBR
202	52	EE
203	91	R/S
204	99	PRT
205	65	×
206	01	1
207	00	0
208	93	.
209	09	9
210	04	4
211	61	GTO
212	99	PRT

Ball check valves

Step	Code	Key
213	76	LBL
214	25	CLR
215	01	1
216	04	4
217	02	2
218	07	7
219	01	1
220	05	5
221	02	2
222	06	6
223	00	0
224	00	0
225	69	OP
226	01	01
227	71	SBR
228	52	EE
229	91	R/S
230	99	PRT
231	65	×
232	01	1
233	02	2
234	93	
235	04	4
236	06	6
237	61	GTO
238	99	PRT

Butterfly valves

Step	Code	Key
239	76	LBL
240	32	X⇌T
241	01	1
242	04	4
243	04	4
244	01	1
245	03	3
246	07	7
247	02	2
248	01	1
249	00	0
250	00	0
251	69	OP
252	01	01
253	71	SBR
254	52	EE
255	91	R/S
256	99	PRT
257	65	×
258	03	3
259	93	.
260	06	6
261	00	0
262	61	GTO
263	99	PRT

3-way straight-through valves

Step	Code	Key
264	76	LBL
265	33	X^2
266	00	0
267	04	4
268	04	4
269	03	3
270	03	3
271	06	6
272	03	3
273	07	7
274	00	0
275	00	0
276	69	OP
277	01	01
278	71	SBR
279	52	EE
280	91	R/S
281	99	PRT
282	65	×
283	03	3
284	93	.
285	06	6
286	07	7
287	61	GTO
288	99	PRT

3-way flow-through branch valves

Step	Code	Key
289	76	LBL
290	34	√X
291	00	0
292	04	4
293	04	4
294	03	3
295	01	1
296	04	4
297	02	2
298	01	1
299	00	0
300	00	0
301	69	OP
302	01	01
303	71	SBR
304	52	EE
305	91	R/S
306	99	PRT
307	65	×
308	01	1
309	01	1
310	93	.
311	06	6
312	07	7
313	61	GTO
314	99	PRT

Long-radius 90-deg. elbows

Step	Code	Key
315	76	LBL
316	13	C
317	02	2
318	07	7
319	03	3
320	05	5
321	01	1
322	02	2
323	00	0
324	01	1
325	00	0
326	00	0
327	69	OP
328	01	01
329	71	SBR
330	65	×
331	91	R/S
332	99	PRT
333	65	×
334	01	1
335	93	.
336	06	6
337	07	7
338	61	GTO
339	99	PRT

Print elbows

Step	Code	Key
340	76	LBL
341	65	×
342	43	RCL
343	23	23
344	69	OP
345	02	02
346	43	RCL
347	24	24
348	69	OP
349	03	03
350	69	OP

Table III

Step	Code	Key
351	05	05
352	92	RTN

Short-radius 90-deg. elbows

Step	Code	Key
353	76	LBL
354	35	1/X
355	03	3
356	06	6
357	03	3
358	05	5
359	01	1
360	02	2
361	00	0
362	01	1
363	00	0
364	00	0
365	69	OP
366	01	01
367	71	SBR
368	65	×
369	91	R/S
370	99	PRT
371	65	×
372	02	2
373	93	.
374	05	5
375	61	GTO
376	99	PRT

Short-radius 45-deg. elbows

Step	Code	Key
377	76	LBL
378	42	STO
379	03	3
380	06	6
381	03	3
382	05	5
383	00	0
384	05	5
385	00	0
386	06	6
387	00	0
388	00	0
389	69	OP
390	01	01
391	71	SBR
392	65	×
393	91	R/S
394	99	PRT
395	65	×
396	01	1
397	93	.
398	03	3
399	03	3
400	61	GTO
401	99	PRT

90-deg. miter bends

Step	Code	Key
402	76	LBL
403	43	RCL
404	01	1
405	02	2
406	00	0
407	01	1
408	00	0
409	00	0
410	03	3
411	00	0
412	02	2
413	04	4
414	69	OP
415	01	01
416	43	RCL
417	25	25
418	69	OP
419	02	02
420	43	RCL
421	26	26
422	69	OP
423	03	03
424	69	OP
425	05	05
426	91	R/S
427	99	PRT
428	65	×
429	04	4
430	93	.
431	08	8
432	03	3
433	61	GTO
434	99	PRT

45-deg. miter bends

Step	Code	Key
435	76	LBL
436	44	SUM
437	00	0
438	05	5
439	00	0
440	06	6
441	00	0
442	00	0
443	03	3
444	00	0
445	02	2
446	04	4
447	69	OP
448	01	01
449	43	RCL
450	25	25
451	69	OP
452	02	02
453	43	RCL
454	26	26
455	69	OP
456	03	03
457	69	OP
458	05	05
459	91	R/S
460	99	PRT
461	65	×
462	01	1
463	93	.
464	02	2
465	05	5
466	61	GTO
467	99	PRT

Straight-through tees

Step	Code	Key
468	76	LBL
469	14	D
470	69	OP
471	00	00
472	03	3
473	06	6
474	03	3
475	07	7
476	00	0
477	00	0
478	03	3
479	07	7
480	01	1
481	07	7
482	69	OP
483	01	01
484	43	RCL
485	27	27
486	69	OP
487	02	02
488	43	RCL
489	18	18
490	69	OP
491	03	03
492	69	OP
493	05	05
494	91	R/S
495	99	PRT
496	65	×
497	01	1
498	93	.
499	06	6
500	07	7
501	61	GTO
502	99	PRT

Flow-through branch tees

Step	Code	Key
503	76	LBL
504	45	Y^x
505	01	1
506	04	4
507	02	2
508	01	1
509	00	0
510	00	0
511	03	3
512	07	7
513	01	1
514	07	7
515	69	OP
516	01	01
517	43	RCL
518	27	27
519	69	OP
520	02	02
521	43	RCL
522	18	18
523	69	OP
524	03	03
525	69	OP
526	05	05
527	91	R/S
528	99	PRT
529	65	×
530	05	5
531	61	GTO
532	99	PRT
533	91	R/S

Reduction/enlargement

Step	Code	Key
534	76	LBL
535	15	E
536	69	OP
537	00	00
538	43	RCL
539	12	12
540	69	OP
541	01	01
542	43	RCL
543	13	13
544	69	OP
545	02	02
546	69	OP
547	05	05
548	02	2
549	01	1
550	03	3
551	07	7
552	69	OP
553	04	04
554	91	R/S
555	99	PRT
556	42	STO
557	19	19
558	43	RCL
559	07	07
560	23	LNX
561	65	×
562	43	RCL
563	14	14
564	85	+
565	43	RCL
566	15	15
567	95	=
568	65	×
569	43	RCL
570	19	19
571	95	=
572	44	SUM
573	00	00
574	69	OP
575	06	06
576	91	R/S

Entrance losses

Step	Code	Key
577	76	LBL
578	16	A'
579	69	OP
580	00	00
581	43	RCL
582	08	08
583	69	OP
584	01	01
585	43	RCL
586	09	09
587	69	OP
588	02	02
589	69	OP
590	05	05
591	02	2
592	01	1
593	03	3
594	07	7
595	69	OP
596	04	04
597	43	RCL
598	07	07
599	45	Y^x
600	43	RCL
601	16	16
602	65	×
603	43	RCL
604	17	17
605	95	=
606	44	SUM
607	00	00
608	69	OP
609	06	06
610	91	R/S

Exit losses

Step	Code	Key
611	76	LBL
612	17	B'
613	69	OP
614	00	00
615	43	RCL
616	10	10
617	69	OP
618	01	01
619	69	OP
620	05	05
621	02	2
622	01	1
623	03	3
624	07	7
625	69	OP
626	04	04
627	43	RCL
628	07	07
629	45	Y^x
630	43	RCL
631	16	16
632	65	×
633	43	RCL
634	17	17
635	65	×
636	02	2
637	95	=
638	44	SUM
639	00	00
640	69	OP
641	06	06
642	91	R/S

Sum of equivalent line lengths

Step	Code	Key
643	76	LBL
644	18	C'
645	69	OP
646	00	00
647	03	3
648	06	6
649	04	4
650	01	1
651	03	3
652	00	0
653	02	2
654	00	0
655	01	1
656	07	7
657	69	OP
658	01	01
659	03	3
660	04	4
661	02	2
662	07	7
663	00	0
664	00	0
665	02	2
666	01	1
667	03	3
668	07	7
669	69	OP
670	02	02
671	69	OP
672	05	05
673	43	RCL
674	00	00
675	99	PRT
676	00	0
677	42	STO
678	00	00
679	91	R/S

Line length

Step	Code	Key
680	76	LBL
681	10	E'
682	00	0
683	42	STO
684	00	00
685	69	OP
686	00	00
687	43	RCL
688	28	28
689	69	OP
690	01	01
691	43	RCL
692	29	29
693	69	OP
694	02	02
695	69	OP
696	05	05
697	91	R/S
698	99	PRT
699	42	STO
700	19	19

(continued next page)

(Continued) Table III

Line length (cont'd)

Step	Code	Key
701	59	INT
702	44	SUM
703	00	00
704	43	RCL
705	19	19
706	22	INV
707	59	INT
708	65	×
709	43	RCL
710	11	11
711	95	=
712	44	SUM
713	00	00
714	61	GTO
715	06	06
716	97	97
717	91	R/S

Label addresses

GATE VALVES	B
GLBE VALVES	INV
PLUG VALVES	LNX
SWCK VALVES	CE
BLCK VALVES	CLR
BUTF VALVES	X⇌T
3WST VALVES	X²
3WBF VALVES	√X
SR90 ELBOWS	1/X
LR90 ELBOWS	C
SR45 ELBOWS	STO
90 MITER BEND	RCL
45 MITER BEND	SUM
ST TEES	D
BF TEES	Y^X
RED/ENLR	E
ENTRANCE	A'

Label addresses (cont'd)

EXIT	B'
SUM-EQL FT	C'
LINE LNGTH	E'

Data registers*

Sum register	00
1734412442.	01
1327173137.	02
27243117.	03
2717312237.	04
2300333532.	05
2235133000.	06
Pipe I.D.	07
1731373513.	08
3115170000.	09
1744243700.	10
8.333333333	11
3517166317.	12
3127350071.	13
2.99761	14
-1.06205	15
1.23787	16
1.83343	17
0.	18
Pipe length	19
4213274217.	20
3600710000.	21
2137.	22
1727143243.	23
3600710000.	24
3717350014.	25
1731160071.	26
1736007100.	27
2724311700.	28
2731223723.	29

*Numbers must be entered

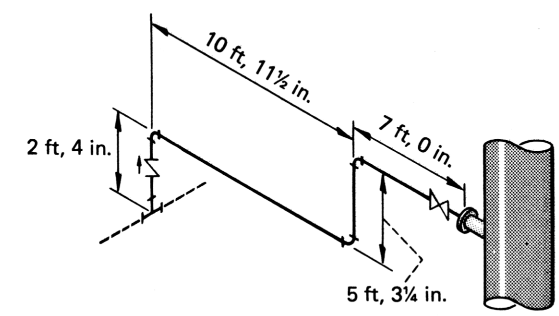
is very convenient and has gained wide acceptance by piping designers for most work. In it, the fitting or valve is taken to be equivalent to so many feet of pipe. By addin^ this calculated length to the line length, the pressure drop for an entire loop can be found at once.

Data from a table of representative equivalent lengths to pipe diameters for various valves and fittings [*1*] were rearranged and expanded by R. Kern [*2*]. Factors for this program were taken from the Kern article. When a single factor was not applicable, an equation was developed to represent the data.

Caution is urged in using the part of the program dealing with piping reduction/enlargement. In most cases, the correlations presented are only valid for $d_1/d_2 < 1.5$. (Negative values may be obtained for very small lines.) For values beyond 1.5, refer to Kern [*2*].

Using the program

Table I gives the program operating instructions and the user-defined keys. Table III provides the program



Piping isometric for the sample calculation

itself, which occupies both sides of two magnetic cards. The partitioning is 719.29. Label addresses and the data that must be stored are also listed in Table III.

After the pipe internal diameter has been keyed in and **R/S** pressed, the subroutine for each type of valve or fitting to be converted is called up. Enter the number of valves or fittings and press **R/S** to calculate the equivalent feet of pipe. After all the valves, fittings, and entrance and exit losses have been converted, the total equivalent length is recalled and printed by pressing **C′**.

To sum pipe lengths, inch dimensions need not be converted into actual equivalents in foot-decimal form. For example, a pipe 12 ft $2\frac{1}{4}$ in. long is entered as 12.0225, and one 2 ft 11 in. long as 2.11.

To begin the pipe-length summing section, first press **E′**. After each pipe length is keyed in as indicated, press **R/S** to convert and store the number. After all the lengths have been entered, press **C′** to obtain the total line length. This feature is also handy for the addition of any linear measurements in feet and inches, such as vessel, tank, tower and plot-plan dimensions.

If a printer is not available, all calculations can still be performed and the totals recalled from storage register **00**. All sums for equivalent lengths of valves, fittings and entrance and exit losses, as well as of line lengths, are stored in this register.

Do not press **C′** to obtain a total without the printer, because register **00** is cleared by the calculator after the sum has been printed. This register is also automatically cleared when either **E′** or **A** is pressed.

Sample problem

A piping isometric (see figure) shows a 4-in. Schedule 40 line containing three 90-deg. long-radius elbows, one flowthrough branch-tee, one gate valve (fully open), one swing check-valve, and an exit loss. The piping section lengths are 2 ft 4 in., 10 ft $11\frac{1}{2}$ in., 7 ft 0 in., and 5 ft $3\frac{1}{4}$ in. What is the total equivalent length?

The calculator printouts are given in Table II. The total equivalent length of the valves, fittings and exit loss is 109 ft. The sum of the line lengths is 26 ft. This yields a total equivalent line length of 135 ft.

For HP-67/97 users

The HP version closely follows the TI program. Table IV contains the HP program listing, and Table V offers user instructions. The HP printout for the example is shown in Table VI.

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	034	1	01	067	3	03	100	×	-35	133	Y^X	31
002	STOA	35 11	035	.	-62	068	.	-62	101	ST+1	35-55 01	134	1	01
003	PRTX	-14	036	6	06	069	6	06	102	PRTX	-14	135	.	-62
004	R/S	51	037	7	07	070	GSB1	23 01	103	R/S	51	136	8	08
005	1	01	038	GSB1	23 01	071	3	03	104	GSB2	23 02	137	3	03
006	.	-62	039	5	05	072	.	-62	105	ST+1	35-55 01	138	3	03
007	6	06	040	GSB1	23 01	073	6	06	106	PRTX	-14	139	4	04
008	7	07	041	1	01	074	7	07	107	R/S	51	140	3	03
009	×	-35	042	.	-62	075	GSB1	23 01	108	GSB2	23 02	141	×	-35
010	RCLA	36 11	043	1	01	076	1	01	109	2	02	142	×	-35
011	×	-35	044	GSB1	23 01	077	1	01	110	×	-35	143	RTN	24
012	STO1	35 01	045	2	02	078	.	-62	111	ST+1	35-55 01	144	*LBLE	21 15
013	PRTX	-14	046	8	08	079	6	06	112	PRTX	-14	145	STOB	35 12
014	R/S	51	047	.	-62	080	7	07	113	RCL1	36 01	146	PRTX	-14
015	2	02	048	3	03	081	GSB1	23 01	114	PRTX	-14	147	INT	16 34
016	.	-62	049	3	03	082	RCLA	36 11	115	R/S	51	148	ST+2	35-55 02
017	5	05	050	GSB1	23 01	083	LN	32	116	*LBL1	21 01	149	RCLB	36 12
018	GSB1	23 01	051	1	01	084	2	02	117	×	-35	150	FRC	16 44
019	1	01	052	.	-62	085	.	-62	118	RCLA	36 11	151	1	01
020	.	-62	053	5	05	086	9	09	119	×	-35	152	2	02
021	3	03	054	GSB1	23 01	087	9	09	120	ST+1	35-55 01	153	÷	-24
022	3	03	055	1	01	088	7	07	121	PRTX	-14	154	1	01
023	GSB1	23 01	056	0	00	089	6	06	122	R/S	51	155	0	00
024	4	04	057	.	-62	090	1	01	123	RTN	24	156	0	00
025	.	-62	058	9	09	091	×	-35	124	*LBL2	21 02	157	×	-35
026	8	08	059	4	04	092	1	01	125	RCLA	36 11	158	ST÷2	35-55 02
027	3	03	060	GSB1	23 01	093	.	-62	126	1	01	159	R/S	51
028	GSB1	23 01	061	1	01	094	6	06	127	.	-62	160	*LBLC	21 13
029	1	01	062	2	02	095	2	02	128	2	02	161	RCL2	36 02
030	.	-62	063	.	-62	096	2	02	129	3	03	162	PRTX	-14
031	2	02	064	4	04	097	6	06	130	7	07	163	R/S	51
032	5	05	065	6	06	098	5	05	131	8	08	164	RTN	24
033	GSB1	23 01	066	GSB1	23 01	099	-	-45	132	7	07	165	R/S	51

User instructions for HP version — Table V

Step	Procedure	Key
1.	Enter pipe diameter, in., then press the **A** key.	**A**
(2.-19.)	Enter the *number* of fittings in each of the following 18 categories and press the **R/S** key after each entry. Where no fittings of a given category are used, enter zero and press the **R/S** key.	
2.	Long radius 90° elbows	**R/S**
3.	Short radius 90° elbows	**R/S**
4.	Short radius 45° elbows	**R/S**
5.	90° miter bends	**R/S**
6.	45° miter bends	**R/S**
7.	Straight-through tees	**R/S**
8.	Flow-through branch tees	**R/S**
9.	Gate valves	**R/S**
10.	Globe valves	**R/S**
11.	Plug valves	**R/S**
12.	Swing check valves	**R/S**
13.	Ball check valves	**R/S**
14.	Butterfly valves	**R/S**
15.	3-way straight-through valves	**R/S**
16.	3-way flow-through branch valves	**R/S**
17.	Reduction/enlargement	**R/S**
18.	Entrance loss	**R/S**
19.	Exit loss	**R/S**
20.	Read the total equivalent lengths.	
21.	Enter each pipe length in ("feet-decimal point-inches"), and after each entry press the **E** key.	**E**
22.	Press the **C** key.	**C**
23.	Read the total pipe length (in decimal feet).	

The printout is in the following order: pipe diameter; equivalent line lengths for each of 18 different types of fitting; total of the listed fitting equivalents; the value, in decimal feet, of each of a series of pipe lengths; and, finally, the total of the pipe lengths.

Example for HP version — Table VI

4.0260 ***	Pipe diameter
20.1703 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
20.1300 ***	
4.4237 ***	
0.0000 ***	Equivalent line lengths for each of the 18 different type of fittings
0.0000 ***	
44.0444 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
0.0000 ***	
20.5612 ***	
109.7345 ***	Total equivalent length
2.0400 ***	
10.1150 ***	
7.0000 ***	Pipe lengths
5.0325 ***	
25.5625 ***	Total pipe length

References

1. "Flow of Fluids," Technical paper No. 410, Crane Co., New York, 1957.
2. Kern, R., How To Compute Pipe Size, *Chem. Eng.*, Jan. 6, 1975, pp. 115–120.

Program predicts pressure drop for gas flow across an orifice meter

Written for the HP-67 or HP-97, this program simplifies calibration of the meter. Also, guidelines are given for constructing and installing this device.

Frank A. Stephens, Amax Specialty Metals Corp.

☐ Most engineers, at one time or another, need to measure the flowrate of a fluid in a pipe. A variety of devices are available to do this. These are often expensive, and frequently have delivery times of weeks or even months.

But long lead times for equipment are often unacceptable. As an alternative, the engineer should consider the use of an orifice meter. Such a meter is easily fabricated in any reasonably equipped machine shop, and can usually be in place in a couple of days.

The reader may remember a weekend spent in college when one's professor assigned the problem of designing an orifice meter to measure the flowrate of a gas stream. It took hours of trial-and-error calculations to determine each point on the curve of flowrate vs. pressure differential across the orifice. Now, however, with the convenience of the small programmable calculators—here, the Hewlett Packard HP-67 or HP-97—the entire flow curve can be generated in the field in less than an hour.

The equation

The calculator program in this article predicts the differential pressure created by an orifice meter at any selected flowrate of a gas (see Table I). In most cases, deviation of the predicted flowrate from the actual will be less than ±3%.

Obviously, before the pressure differential can be predicted, certain parameters pertaining to the orifice meter and the gas stream must be known. These appear in the nomenclature (see box).

The equation used to predict the differential pressure across the orifice for a specific flowrate of gas is:

$$Q = 678YCd_o^2\sqrt{\frac{\Delta PP_1}{T_1S_g}} \qquad (1)$$

This equation, when used in conjunction with the graphs presented here, predicts the maximum pressure drop that can be measured across an orifice. For this reason, vena-contracta taps should be used when applying the method presented in this article. These taps measure the greatest pressure differential.

The value of the expansion factor, Y, in Eq. (1) is determined from the following equation (from Mink [4]):

$$Y = 1 - (0.41 - 0.35\beta^4)\frac{\Delta P}{kP_1} \qquad (2)$$

If the value of $\frac{\Delta P}{kP_1}$ exceeds 0.35, the calculator will display "error." This is because the linear relationship between Y and $\frac{\Delta P}{kP_1}$, as described in Eq. (2), changes at approximately 0.35, and the calculated value of Y may not be accurate.

The value of the coefficient of discharge, C, is obtained from Fig. 1 (from Stearns, et al. [2]). Since the Reynolds number (and therefore the coefficient of discharge) changes with the flowrate of gas, a new coefficient of discharge must be used every time a pressure drop for a given orifice meter is to be determined for a new flowrate of gas.

User's instructions for the program appear in Table II. In Step 11, the calculator may continue to compute for several minutes. When it completes the calculation, it will display the pressure drop across the orifice for five seconds in psi, for the HP-67. Then it will convert the pressure drop to in. H_2O, and leave this number on the display indefinitely. On the HP-97, the answer is printed in psi and displayed in in. H_2O; the psi value is not displayed.

Example

Consider air flowing through a 4-in. pipe at a rate of 175 scfm. Assume that the pipe is equipped with an orifice meter having an inside dia. of 2.4985 in., and that air is at 100°F and 15.486 psia. The following inputs would be made to predict the pressure differential across the orifice:

(Text continues on p. 130)

Originally published November 29, 1982.

Written for the HP-67 or HP-97, program predicts pressure drop for gas flows across orifice meters

Table I

Step	Code	Key
001	*LBLA	21 11
	Inputs $d_o, D, S_g, \mu, k, T_1, P_1$	
002	R/S	51
003	STOC	35 13
004	R/S	51
005	STOD	35 14
006	R/S	51
007	STO3	35 03
008	R/S	51
009	STO2	35 02
010	P⇄S	16-51
011	R/S	51
012	STO1	35 01
013	R/S	51
014	4	04
015	5	05
016	9	09
017	.	-62
018	6	06
019	7	07
020	+	-55
021	STOB	35 12
022	R/S	51
023	STOE	35 15
024	P⇄S	16-51
	Inputs number of decimal points	
025	R/S	51
026	STO1	35 01
027	*LBL5	21 05
028	P⇄S	16-51
	Calc. β	
029	RCLC	36 13
030	RCLD	36 14
031	÷	-24
032	STO2	35 02
033	ENT↑	-21
034	ENT↑	-21
	Calc. "a" in $Y = 1 - a\Delta P$	
035	4	04
036	Y^x	31
037	.	-62
038	3	03
039	5	05
040	x	-35
041	.	-62
042	4	04
043	1	01
044	+	-55
045	RCLE	36 15
046	÷	-24
047	RCL1	36 01
048	÷	-24
049	P⇄S	16-51
050	STO4	35 04
	Displays β	
051	R↓	-31
052	*LBL6	21 06
	Inputs Q	
053	R/S	51
054	STO5	35 05
	Calc. *Re* number	
055	ENT↑	-21
056	2	02
057	8	08
058	.	-62
059	9	09
060	2	02
061	x	-35
062	RCL3	36 03
063	x	-35
064	RCLD	36 14
065	÷	-24
066	RCL2	36 02
067	÷	-24
068	DSP2	-63 02
069	SCI	-12
	Inputs C	
070	R/S	51
071	FIX	-11
072	STO6	35 06
	Calc. "K" in $Q = KY\sqrt{\Delta P}$	
073	6	06
074	7	07
075	8	08
076	RCLC	36 13
077	X^2	53
078	x	-35
079	RCL6	36 06
080	x	-35
081	RCLE	36 15
082	RCLB	36 12
083	÷	-24
084	RCL3	36 03
085	÷	-24
086	√X	54
087	x	-35
088	STO7	35 07
	Formats display; fixes degree of accuracy	
089	RCL1	36 01
090	STOI	35 46
091	DSPi	-63 45
092	3	03
093	+	-55
094	STOI	35 46
	Calc. Q for ΔP_s and ΔP_l (s = smaller, l = larger; program assumes larger or smaller ΔP_s until it converges)	
095	1	01
096	STO0	35 00
097	.	-62
098	0	00
099	0	00
100	1	01
101	STOA	35 11
102	GSB1	23 01
103	STO8	35 08
104	RCL0	36 00
105	RCLA	36 11
106	+	-55
107	STOA	35 11
	Compares Q for ΔP_s and ΔP_l	
108	*LBL2	21 02
109	GSB1	23 01
110	STO9	35 09
111	RCL8	36 08
112	RCL5	36 05
113	-	-45
114	ABS	16 31
115	RCL9	36 09
116	RCL5	36 05
117	-	-45
118	ABS	16 31
119	X>Y?	16-34
120	GTO3	22 03
121	RCL9	36 09
122	STO8	35 08
123	RCL0	36 00
124	RCLA	36 11
125	+	-55
126	X<0?	16-45
127	GTO3	22 03
128	STOA	35 11
129	GTO2	22 02
	Changes the increment	
130	*LBL3	21 03
131	RCL0	36 00
132	1	01
133	0	00
134	CHS	-22
135	÷	-24
136	STO0	35 00
137	RCL9	36 09
138	STO8	35 08
139	DSZI	16 25 46
140	GTO2	22 02
	Checks $\frac{\Delta P}{kP_1} > 0.35$	
141	RCLA	36 11
142	RCLE	36 15
143	÷	-24
144	P⇄S	16-51
145	RCL1	36 01
146	÷	-24
147	P⇄S	16-51
148	.	-62
149	3	03
150	5	05
151	-	-45
152	X>0?	16-44
153	GTO4	22 04
	Outputs ΔP	
154	RCLA	36 11
155	PRTX	-14
156	2	02
157	7	07
158	.	-62
159	7	07
160	0	00
161	7	07
162	x	-35
163	GTO6	22 06
	Subroutine: calc. Q	
164	*LBL1	21 01
165	1	01
166	RCLA	36 11
167	RCL4	36 04
168	x	-35
169	-	-45
170	RCL7	36 07
171	x	-35
172	RCLA	36 11
173	√X	54
174	x	-35
175	RTN	24
	New T_1	
176	*LBLB	21 12
177	4	04
178	5	05
179	9	09
180	.	-62
181	6	06
182	7	07
183	+	-55
184	STOB	35 12
185	GTO5	22 05
	New d_o	
186	*LBLC	21 13
187	STOC	35 13
188	GTO5	22 05
	New D	
189	*LBLD	21 14
190	STOD	35 14
191	GTO5	22 05
	New P_1	
192	*LBLE	21 15
193	STOE	35 15
194	GTO5	22 05
	Display "Error"	
195	*LBL4	21 04
196	0	00
197	÷	-24
198	RTN	24
199	R/S	51

Nomenclature

d_o	Inside dia. of the orifice, in.
D	Inside dia. of pipe, in.
S_g	Specific gravity of gas relative to air, both at standard temperature and pressure
μ	Viscosity of gas at actual temperature and pressure, cP
k	Ratio of specific heats (C_p/C_v) at actual temperature and pressure. Typical values appear in Ref. [1].
T_1	Temperature of gas, R
P_1	Pressure of gas (upstream of orifice plate), psia
Q	Flowrate of gas, scfm (at 60°F, 14.7 psia)
C	Coefficient of discharge

Other parameters, which are not required to be known directly but will be referred to:

Re no.	Reynolds number
β	Orifice-to-pipe-dia. ratio
Y	Expansion factor
ΔP	Differential pressure across orifice, psi

Entry	Variable
press A	—
2.4985	d_o
4.026	D
1.0	S_g
0.023	μ
1.40	k
100	T_1
15.486	P_1
3	No. of decimal points (Output: = 0.62)
175	Q (Output: *Re no.* = 5.47×10^4)
0.667	C from Fig. 1
$\Delta P = 0.141$ psi	
$\Delta P = 3.894$ in. H_2O	

Fabrication/installation

Because the orifice plate is relatively small and its material cost is low, stainless steel is generally the recommended material of construction. Different applica-

User's instructions for running the program **Table II**

Step	Instructions	Input data/units	Keys	Output data
1.	Initiate program.		A	
2.	Enter inside dia. of orifice plate, in.	d_o, in.	R/S	d_o
3.	Enter inside dia. of pipe, in.	D, in.	R/S	D
4.	Enter specific gravity of gas relative to air.	S_g	R/S	S_g
5.	Enter viscosity of gas at flow conditions, cP.	μ, cP	R/S	μ
6.	Enter ratio of specific heats of gas at flow conditions.	k	R/S	k
7.	Enter temperature of gas in °F; calculator will display T_1 in R.	T_1, °F	R/S	T_1, R
8.	Enter pressure of gas upstream of orifice plate, psia.	P_1, psia	R/S	P_1
9.	Enter number of decimal places of accuracy desired (3 are recommended). At this point, the calculator will display β, the ratio of the inside dia. of the orifice to the inside dia. of the pipe. Record the value of β, since it will be needed later to determine the value of the discharge coefficient, C.	No. of decimal points	R/S	β
10.	Enter flowrate of gas at which pressure drop across orifice is to be calculated, scfm. Now the calculator will display the Reynolds number for the gasflow in the pipe. With this Reynolds number and the appropriate value for β, determine the coefficient of discharge from Fig. 1.	Q, scfm	R/S	Reynolds number
11.	Enter value of coefficient of discharge. If $\frac{\Delta P}{kP_1}$ exceeds 0.35, then "error" will be displayed. The value of ΔP for other flowrates may be obtained by proceeding from Step 10. New values of T_1, d_o, D and P_1 may be tried by entering the new value, pressing the appropriate lettered key, and proceeding from Step 10.	C	R/S	ΔP, psi ΔP, in. H_2O

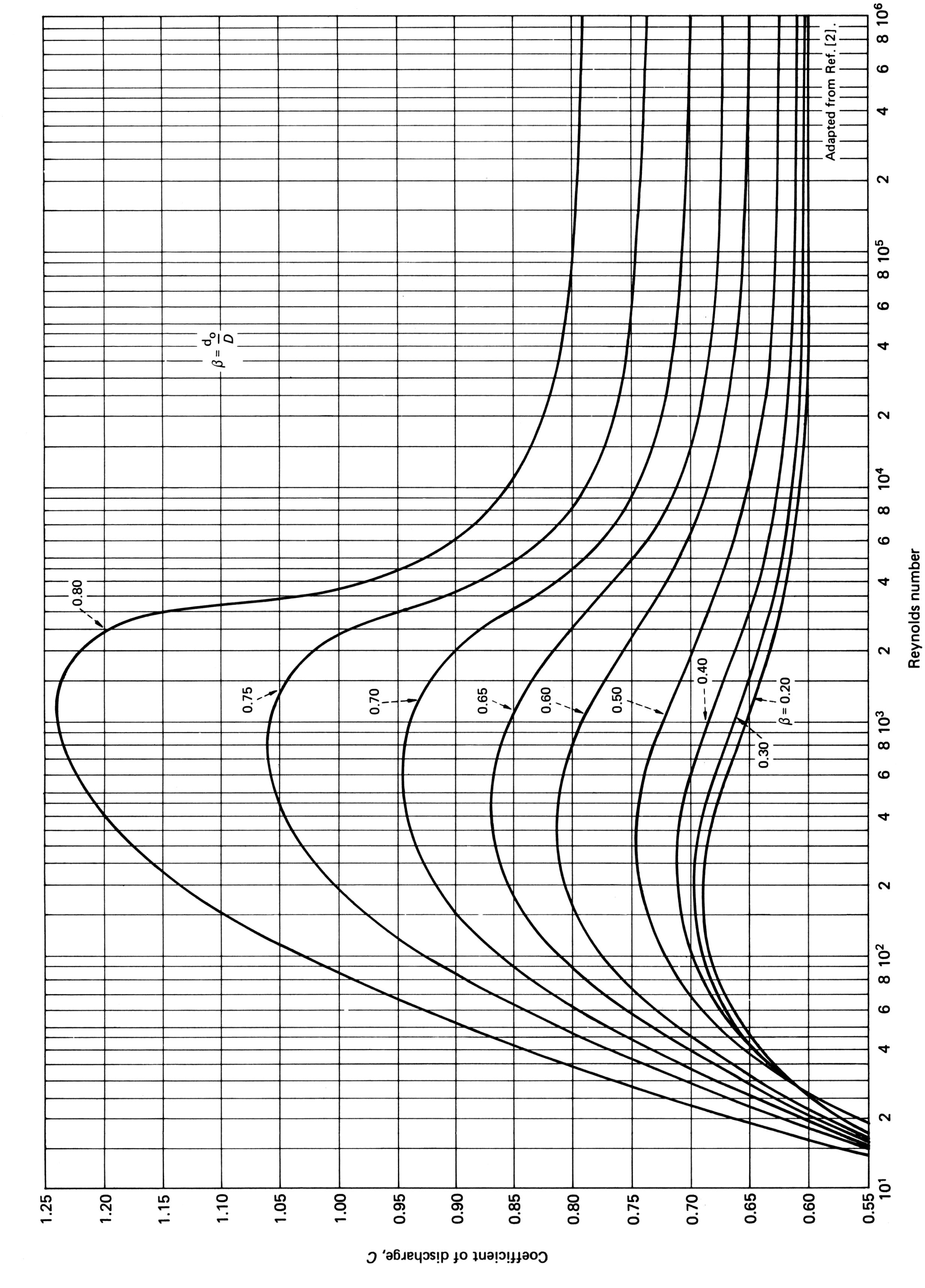


Fig. 1

After the program prints β, the value of C is found from this figure

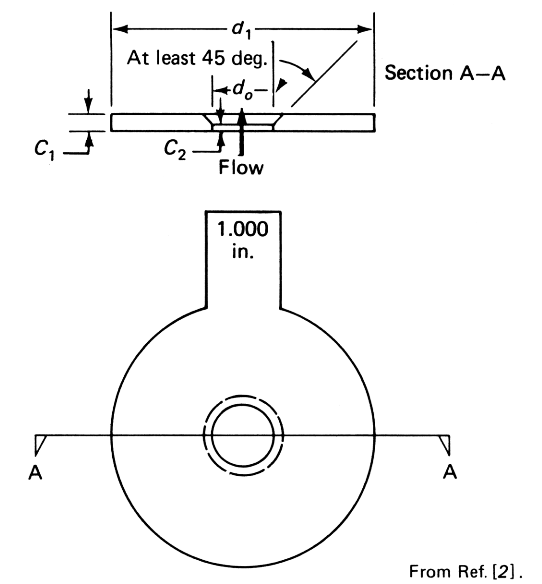
tions may require more-exotic alloys, and the engineer must select the material, depending on each case.

The thickness of the plate depends on the size of the pipe and the differential pressure expected to be applied. The recommended minimum for plate thickness is:

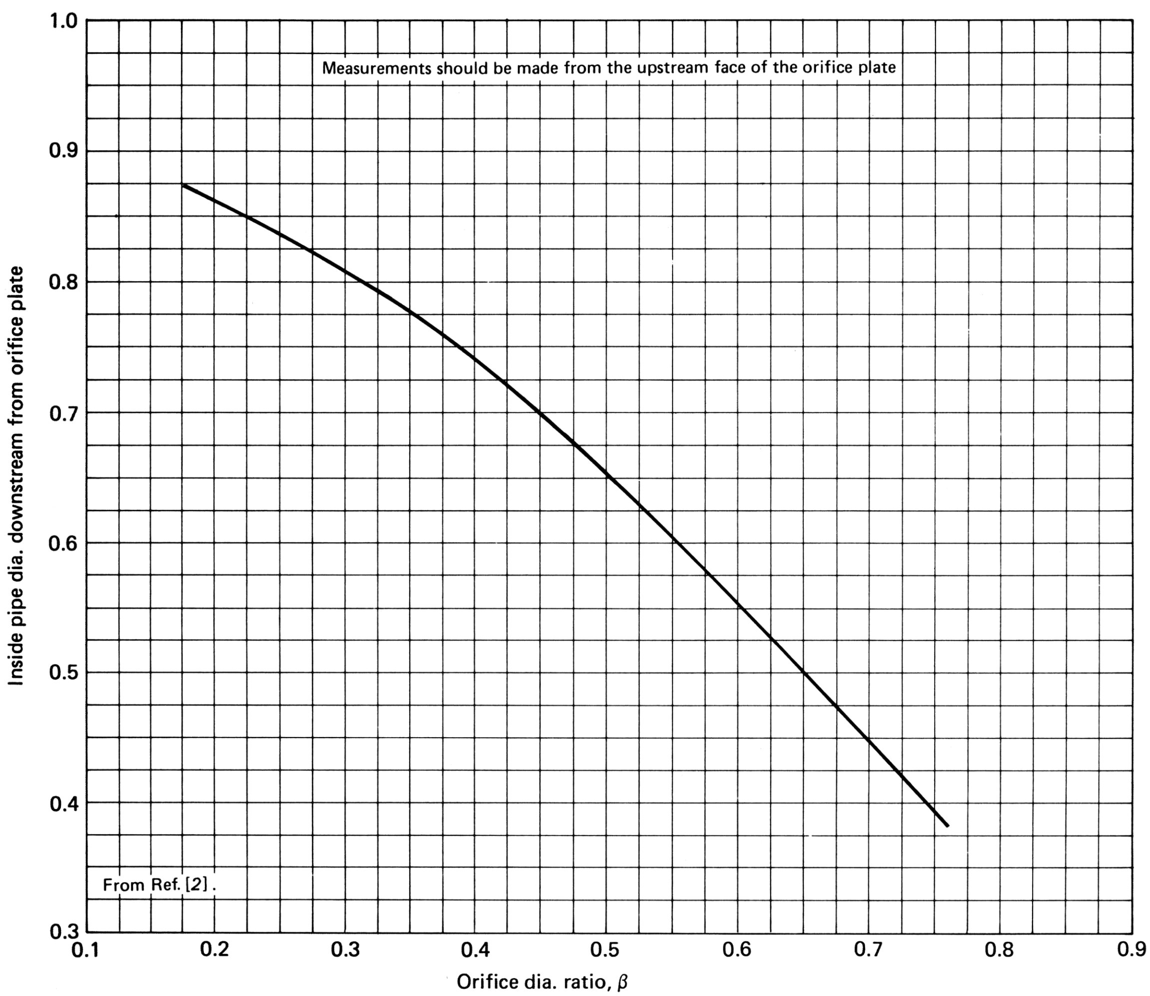
Pipe size, in.	Minimum plate thickness, in.
up to 4	1/16
from 4 to 16	1/8
16 and greater	1/4

Fig. 2 illustrates a typical design for a square-edged orifice plate (from Stearns, et al. [2]). The following rules are suggested guidelines to be used with respect to Fig. 2:

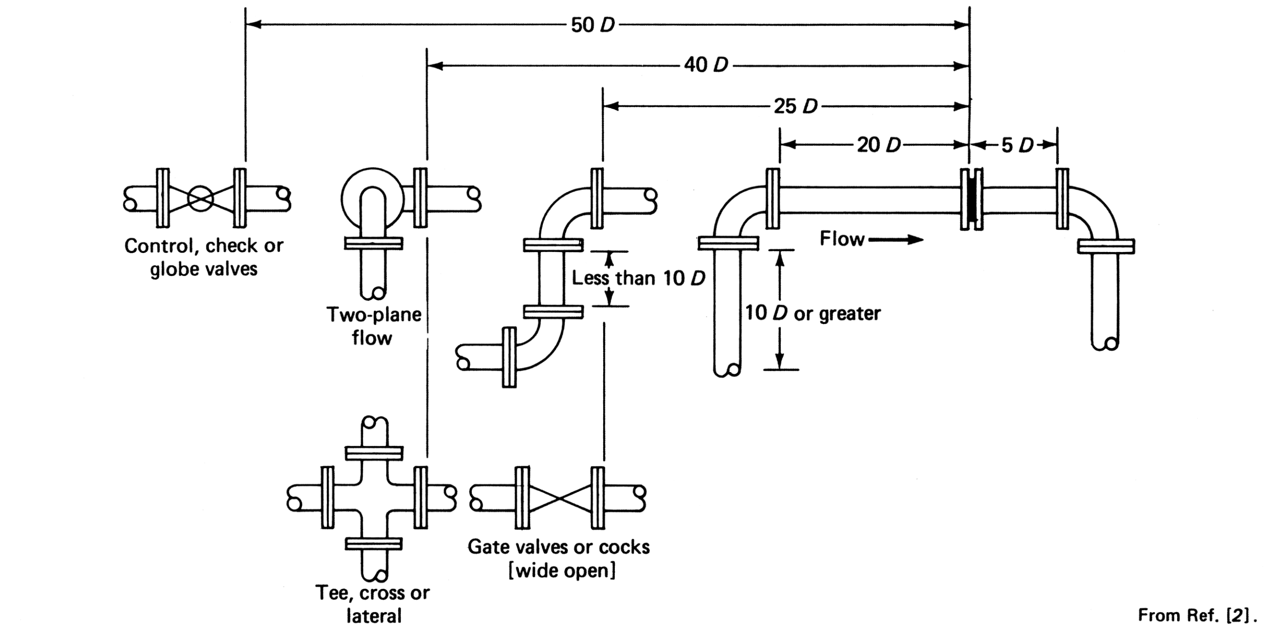
1. The ratio of $\frac{C_2}{d_o}$ should not exceed 0.125 (C_2 is defined in the figure).
2. C_2 should not exceed $1/30$ of the inside pipe dia., D.
3. C_2 should not exceed $1/4$ of $(D - d_o)/2$.
4. β should fall between 0.15 and 0.75 for Reynolds numbers greater than 10,000, and between 0.20 and 0.50 for Reynolds numbers less than 10,000.



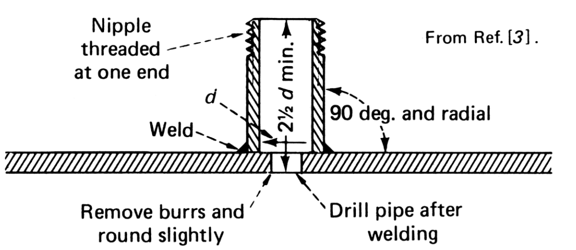
Dimensions for constructing a typical square-edge orifice plate **Fig. 2**



Location of the downstream vena contracta tap depends upon β **Fig. 3**



Selecting the correct piping arrangement ensures accurate measurement **Fig. 4**



Careful design of pipewall pressure taps is needed for accurate data taking **Fig. 5**

5. d_1 should be equal to the diameter of the bolt circle of the flange in which it is to be mounted, minus the diameter of one bolt-hole.

6. In all cases, the leading edge of the orifice plate should be square and sharp.

Locating the taps

Location of the pressure taps can have a dramatic effect on measurement. In order for the measured pressure differential to match the predicted pressure differential, vena-contracta pressure taps should be used, as already mentioned. This means that the center of the upstream tap should be located one inside-pipe-dia. from the upstream face of the orifice plate, and the downstream tap should be located at the point of minimum pressure. Fig. 3 shows the location of point of minimum pressure as a function of the orifice-to-pipe-dia. ratio, β (from Stearns, et al. [2]).

Fig. 5 illustrates a pressure tap used to measure the differential pressure generated by an orifice (from Spink [3]). The recommended diameter of the hole drilled through the wall of the pipe is $\frac{1}{4}$ in. for $2\frac{1}{2}$-in. pipe or smaller; $\frac{3}{8}$ in. for 3 and $3\frac{1}{2}$-in. pipe, and $\frac{1}{2}$ in. for 4-in. pipe and over.

The piping arrangement in which the orifice plate is mounted can also affect the differential pressure, particularly with respect to the upstream piping. Fig. 4 suggests the minimum length of straight pipe that should be installed before and after the orifice plate, depending on the piping arrangement (from Stearns, et al. [2]). All measurements are again made from the upstream face of the plate.

For TI-58/59 users

Table III presents the TI version of the program. User's instructions appear in Table IV, along with the example that was given for the HP version. (Note that, due to roundoff, the TI results differ slightly; the value for the pressure drop for the TI version is 0.140 psi, or 3.871 in. H_2O. Also, the values for the orifice/diameter ratio and the Reynolds number in Table IV have been rounded off; the program yields these values with many more significant figures.)

The decimal has been fixed at 3 places in step 115. The number of places may be changed by simply changing the number in this step.

Program listing for TI version **Table III**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	007	91	R/S	014	42	STO
001	11	A	008	42	STO	015	11	11
002	42	STO	009	03	03	016	91	R/S
003	22	22	010	91	R/S	017	85	+
004	91	R/S	011	42	STO	018	04	4
005	42	STO	012	02	02	019	05	5
006	23	23	013	91	R/S	020	09	9

(Continued) Table III

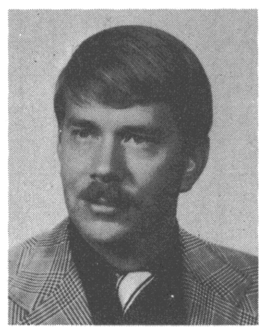
Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
021	93	.	074	65	×	127	42	STO	180	33	X^2	233	01	1
022	06	6	075	43	RCL	128	08	08	181	43	RCL	234	75	−
023	07	7	076	03	03	129	43	RCL	182	00	00	235	43	RCL
024	95	=	077	55	÷	130	00	00	183	55	÷	236	20	20
025	42	STO	078	43	RCL	131	44	SUM	184	01	1	237	65	×
026	21	21	079	23	23	132	20	20	185	00	0	238	43	RCL
027	91	R/S	080	55	÷	133	76	LBL	186	95	=	239	04	04
028	42	STO	081	43	RCL	134	24	CE	187	94	+/-	240	95	=
029	24	24	082	02	02	135	71	SBR	188	42	STO	241	65	×
030	91	R/S	083	95	=	136	23	LNX	189	00	00	242	43	RCL
031	42	STO	084	99	PRT	137	42	STO	190	43	RCL	243	07	07
032	05	05	085	06	6	138	09	09	191	09	09	244	65	×
033	76	LBL	086	42	STO	139	43	RCL	192	42	STO	245	43	RCL
034	22	INV	087	01	01	140	08	08	193	08	08	246	20	20
035	43	RCL	088	91	R/S	141	75	−	194	97	DSZ	247	34	√X
036	22	22	089	42	STO	142	43	RCL	195	01	01	248	95	=
037	55	÷	090	06	06	143	05	05	196	24	CE	249	92	RTN
038	43	RCL	091	65	×	144	95	=	197	00	0	250	76	LBL
039	23	23	092	43	RCL	145	50	I×I	198	32	X⇌T	251	12	B
040	95	=	093	22	22	146	32	X⇌T	199	43	RCL	252	85	+
041	42	STO	094	33	X^2	147	43	RCL	200	20	20	253	04	4
042	12	12	095	65	×	148	09	09	201	55	÷	254	05	5
043	43	RCL	096	06	6	149	75	−	202	43	RCL	255	09	9
044	12	12	097	07	7	150	43	RCL	203	24	24	256	93	.
045	99	PRT	098	08	8	151	05	05	204	55	÷	257	06	6
046	45	Y^X	099	65	×	152	95	=	205	43	RCL	258	07	7
047	04	4	100	53	(	153	50	I×I	206	11	11	259	95	=
048	65	×	101	43	RCL	154	67	EQ	207	75	−	260	42	STO
049	93	.	102	24	24	155	44	SUM	208	93	.	261	21	21
050	03	3	103	55	÷	156	77	GE	209	03	3	262	61	GTO
051	05	5	104	43	RCL	157	33	X^2	210	05	5	263	22	INV
052	85	+	105	21	21	158	76	LBL	211	95	=	264	76	LBL
053	93	.	106	55	÷	159	44	SUM	212	67	EQ	265	13	C
054	04	4	107	43	RCL	160	43	RCL	213	45	Y^X	266	42	STO
055	01	1	108	03	03	161	09	09	214	77	GE	267	22	22
056	95	=	109	54	)	162	42	STO	215	52	EE	268	61	GTO
057	55	÷	110	34	√X	163	08	08	216	76	LBL	269	22	INV
058	43	RCL	111	95	=	164	00	0	217	45	Y^X	270	76	LBL
059	24	24	112	42	STO	165	32	X⇌T	218	43	RCL	271	14	D
060	55	÷	113	07	07	166	43	RCL	219	20	20	272	42	STO
061	43	RCL	114	58	FIX	167	00	00	220	99	PRT	273	23	23
062	11	11	115	03	03	168	85	+	221	65	×	274	61	GTO
063	95	=	116	01	1	169	43	RCL	222	02	2	275	22	INV
064	42	STO	117	42	STO	170	20	20	223	07	7	276	76	LBL
065	04	04	118	00	00	171	95	=	224	93	.	277	15	E
066	43	RCL	119	93	.	172	22	INV	225	07	7	278	42	STO
067	05	05	120	00	0	173	77	GE	226	00	0	279	24	24
068	65	×	121	00	0	174	33	X^2	227	07	7	280	61	GTO
069	02	2	122	01	1	175	42	STO	228	95	=	281	22	INV
070	08	8	123	42	STO	176	20	20	229	99	PRT			
071	93	.	124	20	20	177	61	GTO	230	91	R/S			
072	09	9	125	71	SBR	178	24	CE	231	76	LBL			
073	02	2	126	23	LNX	179	76	LBL	232	23	LNX			

User's instructions for the TI version **Table IV**

Step	Instructions	Input data/units	Value	Keys	Output data
1.	Enter the program.				
2.	Enter inside diameter of orifice plate, in.	d_o, in.	2.4985	A	d_o
3.	Enter inside diameter of pipe, in.	D, in.	4.026	R/S	D
4.	Enter specific gravity of gas relative to air.	S_g	1.0	R/S	S_g
5.	Enter viscosity of gas at flow conditions, cP.	μ, cP	0.023	R/S	μ
6.	Enter ratio of specific heats of gas at flow conditions.	k	1.40	R/S	k
7.	Enter temperature of gas in °F; calculator will display T_1 in R.	T_1,°F	100	R/S	T_1
8.	Enter pressure of gas upstream of orifice plate, psia.	P_1,psia	15.486	R/S	P_1
9.	Enter flowrate of gas at which pressure drop across orifice is to be calculated, scfm. Now the calculator will display β and the Reynolds number for the gasflow in the pipe. With this Reynolds number and the appropriate value for β, determine the coefficient of discharge from Fig. 1.	Q, scfm	175	R/S	0.6206 β 54,656 *Re*
10.	Enter value of coefficient of discharge.	C	0.667	R/S	0.140 ΔP, psi 3.871 ΔP, in. H_2O
	If $\frac{\Delta P}{kP_1}$ exceeds 0.35, then "error" will be displayed.				
	The value of ΔP for other flowrates may be obtained by proceeding from step 2.				

References

1. Perry, R. H., and Chilton, C. H., "Chemical Engineers' Handbook," 5th ed., McGraw-Hill Book Co., New York, 1973, p. 3-134.
2. Stearns, R. F., et al., "Flow Measurement with Orifice Meters," D. Van Nostrand Co., New York, 1951.
3. Spink, L. K., "Principles and Practice of Flow Meter Engineering," 8th ed., The Foxboro Co., Foxboro, Mass., 1958.
4. Mink, W. H., Program Calculates Orifice Sizes for Gas Flows, *Chem. Eng.*, Aug. 25, 1980, Vol. 87, No. 17, p. 91.



The author

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Section V
Heat Transfer

Calculator program for a steam condenser

This program calculates the weighted mean-temperature-difference between the fluids inside and outside the tubes of a steam condenser and the saturation temperature of the steam-vapor mixture as well as the various heat loads.

Larry J. Haydu, Kennecott Engineering Systems Co.

☐ There are three loads in a heat exchanger used for condensing steam out of a noncondensable vapor—gas cooling, condensing, and liquid subcooling.

In order to select the correct cooler/condenser for a particular job, it is necessary to determine the heat load distribution and the overall weighted mean-temperature-difference.

$$\text{Wtd. MTD} = Q_t/[\Sigma(Q_i/\Delta T_i)]$$

where Q_t = total heat load

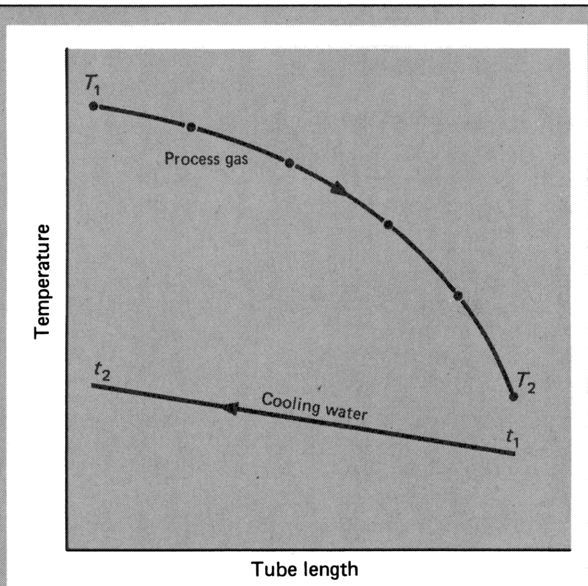
Q_i = incremental heat load over a selected interval

ΔT_i = log MTD for that interval

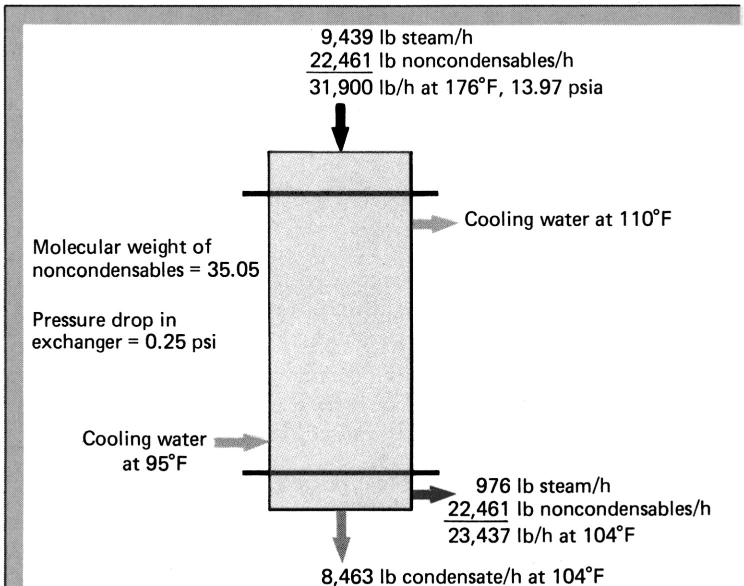
The program

Written for the Hewlett-Packard HP-67/97, the program (Table I) has these main features:

1. The saturation (dewpoint) temperature of the steam-vapor mixture is calculated.
2. The amount of steam condensed in the exchanger is determined.
3. The gas-cooling, condensing, and liquid-subcooling heat loads are calculated, including any desuperheating that occurs above the saturation temperature.
4. An overall weighted MTD is determined, based on the heat-load distribution. Weighted MTDs for the unsaturated and saturated zones are also calculated.



Heat release curve Fig. 1



Steam condenser example Fig. 2

Originally published February 9, 1981.

Calculator program for a steam condenser

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
	Part I		035	3	03	071	X⇄Y	-41	107	÷	-24	141	2	02
	Side 1		036	8	08	072	-	-45	108	RCLA	36 11	142	÷	-24
001	*LBLA	21 11	037	1	01	073	STOE	35 15	109	X⇄Y	-41	143	RCLE	36 15
002	RCL9	36 09	038	.	-62	074	*LBLB	21 12	110	÷	-24	144	+	-55
003	5	05	039	3	03	075	2	02	111	RCLA	36 11	145	4	04
004	÷	-24	040	-	-45	076	STOI	35 46	112	-	-45	146	6	06
005	STO9	35 09	041	STOE	35 15	077	*LBLC	21 13		**Part I**		147	0	00
006	RCL1	36 01	042	PSE	16 51	078	RCL4	36 04		**Side 2**		148	+	-55
007	RCL2	36 02	043	RCL5	36 05	079	RCL9	36 09	113	1	01	149	1	01
008	÷	-24	044	X≤Y?	16-35	080	-	-45	114	8	08	150	1	01
009	STOA	35 11	045	GTOb	22 16 12	081	STO4	35 04	115	×	-35	151	6	06
010	RCL0	36 00	046	-	-45	082	RCLE	36 15	116	RCL0	36 00	152	5	05
011	STOB	35 12	047	CHS	-22	083	CHS	-22	117	X⇄Y	-41	153	.	-62
012	1	01	048	STOD	35 14	084	3	03	118	STO8	35 08	154	1	01
013	8	08	049	GSBa	23 16 11	085	8	08	119	-	-45	155	X⇄Y	-41
014	÷	-24	050	ST+1	35-55 01	086	1	01	120	STOC	35 13	156	-	-45
015	+	-55	051	P⇄S	16-51	087	.	-62	121	2	02	157	4	04
016	LSTX	16-63	052	RCLE	36 15	088	3	03	122	÷	-24	158	9	09
017	X⇄Y	-41	053	RCL6	36 06	089	-	-45	123	P⇄S	16-51	159	3	03
018	÷	-24	054	-	-45	090	3	03	124	RCL0	36 00	160	.	-62
019	RCL4	36 04	055	5	05	091	0	00	125	+	-55	161	1	01
020	×	-35	056	÷	-24	092	2	02	126	RCLD	36 14	162	÷	-24
021	LOG	16 32	057	STOD	35 14	093	7	07	127	×	-35	163	.	-62
022	CHS	-22	058	RCLE	36 15	094	X⇄Y	-41	128	ST+9	35-55 09	164	3	03
023	6	06	059	X⇄Y	-41	095	÷	-24	129	ST+i	35-55 45	165	8	08
024	.	-62	060	-	-45	096	6	06	130	RCLC	36 13	166	Y^x	31
025	2	02	061	STOE	35 15	097	.	-62	131	ST+0	35-55 00	167	9	09
026	6	06	062	GTOB	22 12	098	2	02	132	P⇄S	16-51	168	7	07
027	7	07	063	*LBLb	21 16 12	099	6	06	133	2	02	169	0	00
028	+	-55	064	RCL5	36 05	100	7	07	134	÷	-24	170	.	-62
029	3	03	065	RCL6	36 06	101	+	-55	135	RCL0	36 00	171	3	03
030	0	00	066	-	-45	102	10^x	16 33	136	+	-55	172	×	-35
031	2	02	067	5	05	103	RCL4	36 04	137	STOB	35 12	173	RCLC	36 13
032	7	07	068	÷	-24	104	X⇄Y	-41	138	GSBa	23 16 11	174	×	-35
033	X⇄Y	-41	069	STOD	35 14	105	-	-45	139	ST+i	35-55 45	175	ST+8	35-55 08
034	÷	-24	070	RCL5	36 05	106	RCL4	36 04	140	RCLD	36 14	176	ST+i	35-55 45

Calculation of the weighted MTD depends on the shape of the heat-release curve [*1,2*]. This curve indicates the amount of heat transfer at a given temperature as the gas is cooled and steam condenses out. A greater percentage of steam condenses just below the dewpoint than at lower temperatures, so the heat load per unit temperature drop is higher, giving the figure its curved shape (Fig. 1).

For calculation purposes, the heat-release curve is broken into several zones, so that when straight lines are drawn between the different points they will approximate the curve. The weighted MTD is then obtained by computing the logarithmic mean-temperature-difference between the vapor and coolant temperatures over the intervals of the condensing range. The equations are shown in Table II. It is assumed for the sake of this article that the vapor and coolant always flow countercurrently.

The program is in two parts and stored on two cards. Part I calculates the heat load over the condensing temperature range in five successive steps. For each temperature interval, the gas-cooling, condensing, and liquid-subcooling heat duties are computed and accumulated in separate memory registers. If the steam is unsaturated at the inlet, a sixth temperature interval is

Nomenclature

Symbol	Item	Units
HS	Saturation humidity	lb steam/lb noncondensables
HV	Latent heat of vaporization	Btu/lb
M_a	Molecular weight of steam	eighteen lb/lb mole
M_b	Molecular weight of noncondensables	lb/lb mole
MTD	Mean-temperature-difference	°F
P_a	Partial pressure of steam	psi
P_t	Total pressure	psia
Q_c	Heat of condensation	Btu/h
Q_g	Heat of gas cooling	Btu/h
Q_i	Incremental heat load	Btu/h
Q_l	Heat of liquid subcooling	Btu/h
Q_t	Total heat load	Btu/h
T	Temperature of vapor	°F
t	Temperature of coolant	°F
T_c	Critical temperature of water	1,165.1°R
ΔT_i	Log mean-temperature-difference	°F
VP	Vapor pressure of steam	psi

Table I

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
	Side 2		211	ST+7	35-55 07	032	RCL1	36 01	068	ISZI	16 26 46	104	LN	32
	(cont'd)		212	RTN	24	033	RCLE	36 15	069	RCL2	36 02	105	÷	-24
177	RCLE	36 15	213	R/S	51	034	×	-35	070	STO1	35 01	106	F2?	16 23 02
178	RCLD	36 14		**Part II**		035	P⇄S	16-51	071	RCLD	36 14	107	STOC	35 13
179	-	-45		**Side 1**		036	RCL8	36 08	072	-	-45	108	P⇄S	16-51
180	STOE	35 15	001	*LBLA	21 11	037	X⇄Y	-41	073	STO2	35 02	109	RCLi	36 45
181	P⇄S	16-51	002	P⇄S	16-51	038	-	-45	074	RCL4	36 04	110	X⇄Y	-41
182	ISZI	16 26 46	003	RCL7	36 07	039	STO4	35 04	075	STO3	35 03	111	÷	-24
183	6	06	004	RCL8	36 08	040	GSBD	23 14	076	6	06	112	ST+0	35-55 00
184	RCLI	36 46	005	+	-55	041	SF2	16 21 02	077	RCLI	36 46		**Part II**	
185	X≤Y?	16-35	006	RCL9	36 09	042	RCLB	36 12	078	X≤Y?	16-35		**Side 2**	
186	GTOC	22 13	007	+	-55	043	STO1	35 01	079	GTOC	22 13	113	P⇄S	16-51
187	RCL0	36 00	008	STOA	35 11	044	2	02	080	P⇄S	16-51	114	RTN	24
188	RCL1	36 01	009	P⇄S	16-51	045	STOI	35 46	081	RCLA	36 11	115	*LBLE	21 15
189	+	-55	010	RCL8	36 08	046	GTOC	22 13	082	RCL0	36 00	116	RCLC	36 13
190	P⇄S	16-51	011	STO3	35 03	047	*LBLB	21 12	083	÷	-24	117	÷	-24
191	RCL7	36 07	012	RCL7	36 07	048	STO1	35 01	084	STOE	35 15	118	RCL0	36 00
192	RCL8	36 08	013	-	-45	049	2	02	085	STOD	35 14	119	X⇄Y	-41
193	+	-55	014	X⇄Y	-41	050	STOI	35 46	086	RCL1	36 01	120	-	-45
194	RCL9	36 09	015	÷	-24	051	0	00	087	X>0?	16-44	121	RCLA	36 11
195	+	-55	016	STOE	35 15	052	STOC	35 13	088	GSBE	23 15	122	RCL1	36 01
196	P⇄S	16-51	017	1	01	053	*LBLC	21 13	089	RCLE	36 15	123	-	-45
197	RTN	24	018	STOI	35 46	054	RCL1	36 01	090	RTN	24	124	X⇄Y	-41
198	*LBLa	21 16 11	019	RCLD	36 14	055	RCLD	36 14	091	*LBLD	21 14	125	÷	-24
199	RCL1	36 01	020	5	05	056	-	-45	092	RCL1	36 01	126	STOD	35 14
200	RCL3	36 03	021	×	-35	057	STO2	35 02	093	RCL4	36 04	127	RTN	24
201	×	-35	022	RCL6	36 06	058	P⇄S	16-51	094	-	-45	128	R/S	51
202	RCLB	36 12	023	+	-55	059	RCLi	36 45	095	STO0	35 00			
203	.	-62	024	STOB	35 12	060	RCLE	36 15	096	RCL2	36 02			
204	4	04	025	RCL5	36 05	061	×	-35	097	RCL3	36 03			
205	5	05	026	X≤Y?	16-35	062	P⇄S	16-51	098	-	-45			
206	×	-35	027	GTOB	22 12	063	RCL3	36 03	099	STO9	35 09			
207	+	-55	028	STO1	35 01	064	X⇄Y	-41	100	-	-45			
208	RCLD	36 14	029	X⇄Y	-41	065	-	-45	101	RCL0	36 00			
209	×	-35	030	STO2	35 02	066	STO4	35 04	102	RCL9	36 09			
210	P⇄S	16-51	031	P⇄S	16-51	067	GSBD	23 14	103	÷	-24			

Equations used in the calculations **Table II**

		Ref.
Antoine equation for vapor pressure of steam	$\log VP = C_1/(T + C_2) + C_3$	(4)
	Constants $C_1 = -3{,}027$	
	$C_2 = 381.3$	
	$C_3 = 6.267$	
Watson equation for heat of vaporization	$HV_2 = HV_1[(T_c - T_2)/(T_c - T_1)]^{0.38}$	(3)
Saturation humidity	$HS = \dfrac{M_a P_a}{M_b (P_t - P_a)}$	(5)
Weighted mean-temperature-difference	$\text{Wtd MTD} = \dfrac{Q_t}{\Sigma Q_i/\Delta T_i}$	(1,2)
Log mean-temperature-difference	$\Delta T_i = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln[(T_1 - t_2)/(T_2 - t_1)]}$	(1,2)
Total heat load	$Q_t = Q_g + Q_c + Q_l$	(1,2)
Specific heat of steam	0.45 Btu/lb °F	
Specific heat of water	1.0 Btu/lb °F	

Temperatures in the Watson equation are in °R; all other temperatures are in °F.

User's instructions and sample calculations **Table III**

Step	Value	Example	Key
1. Clear primary and secondary registers			CL REG
			P⇌S
			CL REG
2. Store input data in primary registers			
	Steam inlet rate, lb/h	9,439	STO 0
	Noncondensable rate, lb/h	22,461	STO 1
	Molecular weight noncond., lb/lb mole	35.05	STO 2
	Specific heat inerts, Btu/lb °F	0.22	STO 3
	Operating pressure, absolute psia	13.97	STO 4
	Inlet gas temperature, °F	176	STO 5
	Outlet gas temperature, °F	104	STO 6
	Coolant inlet temperature, °F	95	STO 7
	Coolant outlet temperature, °F	110	STO 8
	Pressure drop of vapor, psi	0.25	STO 9
3. Load program Part I, sides 1 and 2			
4. Begin computations			A
5. Program pauses (briefly) to display saturation temperature, °F		172.23	
6. Recall output from primary and secondary registers			
	Q (total), Btu/h	9,463,302.32	Display
	Steam rate out, lb/h	976.26	RCL 0
			P⇌S
	Steam condensed, lb/h	8,462.74	RCL 0
	Q (gas cool) incl. desuperheat, Btu/h	483,665.53	RCL 7
	Q (condensed), Btu/h	8,584,213.88	RCL 8
	Q (liquid subcool), Btu/h	395,422.92	RCL 9
	Q (desuperheat), Btu/h	34,659.50	RCL 1
7. Return to primary registers			P⇌S
8. Load program Part II, sides 1 and 2			
9. Begin computations			A
10. Recall output			
	Overall weighted MTD, °F	37.60	Display
	Wtd. MTD saturation zone, °F	37.55	RCL D
	Wtd. MTD unsaturated zone, °F	57.97	RCL C
	Saturation temperature, °F	172.23	RCL B

used to figure the heat of desuperheating the steam-vapor mixture. The Watson analogy [*3*] is used to calculate the heat of vaporization for water (Table II). The Antoine equation [*4*] is used to predict the vapor pressure of steam.

Part II calculates the weighted MTD from the information in Part I. Individual MTDs are also figured for the desuperheated and saturated zones.

An example is illustrated in Fig. 2, and a step-by-step procedure for using the program is detailed in Table III.

For TI-58/59 users

The TI version of the program has two parts, program A and program B, (for listings, see Tables IV and V). Table VI contains user instructions and the same example that was given for the HP version.

Listing for TI version—program A **Table IV**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	015	42	STO	030	43	RCL
001	11	A	016	20	20	031	00	00
002	43	RCL	017	43	RCL	032	55	÷
003	09	09	018	00	00	033	01	1
004	55	÷	019	42	STO	034	08	8
005	05	5	020	21	21	035	85	+
006	95	=	021	53	(	036	43	RCL
007	42	STO	022	53	(	037	20	20
008	09	09	023	43	RCL	038	54	)
009	43	RCL	024	00	00	039	65	×
010	01	01	025	55	÷	040	43	RCL
011	55	÷	026	01	1	041	04	04
012	43	RCL	027	08	8	042	54	)
013	02	02	028	55	÷	043	28	LOG
014	95	=	029	53	(	044	75	-

(Continued) Table IV

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
045	06	6	108	43	RCL	171	75	-	234	42	STO	297	44	SUM
046	93	.	109	05	05	172	43	RCL	235	21	21	298	25	25
047	02	2	110	75	-	173	36	36	236	71	SBR	299	43	RCL
048	06	6	111	43	RCL	174	54	)	237	23	LNX	300	25	25
049	07	7	112	06	06	175	35	1/X	238	43	RCL	301	32	X⇄T
050	54	)	113	95	=	176	65	×	239	39	39	302	01	1
051	55	÷	114	55	÷	177	43	RCL	240	74	SM*	303	06	6
052	03	3	115	05	5	178	20	20	241	25	25	304	77	GE
053	00	0	116	95	=	179	65	×	242	43	RCL	305	13	C
054	02	2	117	42	STO	180	43	RCL	243	23	23	306	43	RCL
055	07	7	118	23	23	181	04	04	244	55	÷	307	17	17
056	94	+/-	119	43	RCL	182	75	-	245	02	2	308	85	+
057	95	=	120	05	05	183	43	RCL	246	85	+	309	43	RCL
058	35	1/X	121	75	-	184	20	20	247	43	RCL	310	18	18
059	75	-	122	43	RCL	185	95	=	248	24	24	311	85	+
060	03	3	123	23	23	186	65	×	249	85	+	312	43	RCL
061	08	8	124	95	=	187	01	1	250	04	4	313	19	19
062	01	1	125	42	STO	188	08	8	251	06	6	314	95	=
063	93	.	126	24	24	189	95	=	252	00	0	315	99	PRT
064	03	3	127	76	LBL	190	42	STO	253	95	=	316	43	RCL
065	95	=	128	12	B	191	40	40	254	94	+/-	317	00	00
066	42	STO	129	01	1	192	43	RCL	255	85	+	318	99	PRT
067	24	24	130	02	2	193	00	00	256	01	1	319	43	RCL
068	99	PRT	131	42	STO	194	75	-	257	01	1	320	10	10
069	43	RCL	132	25	25	195	43	RCL	258	06	6	321	99	PRT
070	05	05	133	76	LBL	196	40	40	259	05	5	322	43	RCL
071	32	X⇄T	134	13	C	197	95	=	260	93	.	323	17	17
072	43	RCL	135	43	RCL	198	42	STO	261	01	1	324	99	PRT
073	24	24	136	09	09	199	22	22	262	95	=	325	43	RCL
074	77	GE	137	22	INV	200	43	RCL	263	55	÷	326	18	18
075	22	INV	138	44	SUM	201	40	40	264	04	4	327	99	PRT
076	32	X⇄T	139	04	04	202	42	STO	265	09	9	328	43	RCL
077	75	-	140	03	3	203	00	00	266	03	3	329	19	19
078	43	RCL	141	00	0	204	43	RCL	267	93	.	330	99	PRT
079	24	24	142	02	2	205	22	22	268	01	1	331	43	RCL
080	95	=	143	07	7	206	55	÷	269	95	=	332	11	11
081	42	STO	144	94	+/-	207	02	2	270	45	Y^X	333	99	PRT
082	23	23	145	55	÷	208	85	+	271	93	.	334	91	R/S
083	71	SBR	146	53	(	209	43	RCL	272	03	3	335	76	LBL
084	23	LNX	147	43	RCL	210	10	10	273	08	8	336	23	LNX
085	43	RCL	148	24	24	211	95	=	274	95	=	337	43	RCL
086	39	39	149	85	+	212	65	×	275	65	×	338	01	01
087	44	SUM	150	03	3	213	43	RCL	276	43	RCL	339	65	×
088	11	11	151	08	8	214	23	23	277	22	22	340	43	RCL
089	43	RCL	152	01	1	215	95	=	278	65	×	341	03	03
090	24	24	153	93	.	216	42	STO	279	09	9	342	85	+
091	75	-	154	03	3	217	38	38	280	07	7	343	53	(
092	43	RCL	155	54	)	218	44	SUM	281	00	0	344	43	RCL
093	06	06	156	85	+	219	19	19	282	93	.	345	21	21
094	95	=	157	06	6	220	74	SM*	283	03	3	346	65	×
095	55	÷	158	93	.	221	25	25	284	95	=	347	93	.
096	05	5	159	02	2	222	43	RCL	285	42	STO	348	04	4
097	95	=	160	06	6	223	22	22	286	37	37	349	05	5
098	42	STO	161	07	7	224	44	SUM	287	44	SUM	350	54	)
099	23	23	162	54	)	225	10	10	288	18	18	351	95	=
100	43	RCL	163	95	=	226	43	RCL	289	74	SM*	352	65	×
101	23	23	164	22	INV	227	22	22	290	25	25	353	43	RCL
102	22	INV	165	28	LOG	228	55	÷	291	43	RCL	354	23	23
103	44	SUM	166	42	STO	229	02	2	292	23	23	355	95	=
104	24	24	167	36	36	230	85	+	293	22	INV	356	42	STO
105	12	B	168	53	(	231	43	RCL	294	44	SUM	357	39	39
106	76	LBL	169	43	RCL	232	00	00	295	24	24	358	44	SUM
107	22	INV	170	04	04	233	95	=	296	01	1	359	17	17
												360	92	RTN

Listing for TI version—program B **Table V**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	056	21	21	111	75	-	166	77	GE	221	35	35
001	11	A	057	42	STO	112	53	(	167	33	X^2	222	22	INV
002	43	RCL	058	02	02	113	73	RC*	168	76	LBL	223	87	IFF
003	17	17	059	43	RCL	114	25	25	169	32	X⇌T	224	02	02
004	85	+	060	08	08	115	65	×	170	43	RCL	225	35	1/X
005	43	RCL	061	75	-	116	43	RCL	171	24	24	226	43	RCL
006	18	18	062	53	(	117	24	24	172	99	PRT	227	35	35
007	85	+	063	43	RCL	118	54	)	173	43	RCL	228	42	STO
008	43	RCL	064	11	11	119	95	=	174	23	23	229	22	22
009	19	19	065	65	×	120	42	STO	175	99	PRT	230	22	INV
010	95	=	066	43	RCL	121	04	04	176	43	RCL	231	86	STF
011	42	STO	067	24	24	122	71	SBR	177	22	22	232	02	02
012	20	20	068	54	)	123	23	LNX	178	99	PRT	233	76	LBL
013	43	RCL	069	95	=	124	01	1	179	43	RCL	234	35	1/X
014	08	08	070	42	STO	125	44	SUM	180	21	21	235	73	RC*
015	42	STO	071	04	04	126	25	25	181	99	PRT	236	25	25
016	03	03	072	71	SBR	127	43	RCL	182	91	R/S	237	55	÷
017	53	(	073	23	LNX	128	02	02	183	76	LBL	238	43	RCL
018	43	RCL	074	86	STF	129	42	STO	184	23	LNX	239	35	35
019	08	08	075	02	02	130	01	01	185	43	RCL	240	85	+
020	75	-	076	43	RCL	131	43	RCL	186	01	01	241	43	RCL
021	43	RCL	077	21	21	132	01	01	187	75	-	242	10	10
022	07	07	078	42	STO	133	75	-	188	43	RCL	243	95	=
023	54	)	079	01	01	134	43	RCL	189	04	04	244	42	STO
024	55	÷	080	01	1	135	23	23	190	95	=	245	10	10
025	43	RCL	081	02	2	136	95	=	191	42	STO	246	92	RTN
026	20	20	082	42	STO	137	42	STO	192	00	00	247	76	LBL
027	95	=	083	25	25	138	02	02	193	43	RCL	248	33	X^2
028	42	STO	084	61	GTO	139	43	RCL	194	02	02	249	53	(
029	24	24	085	24	CE	140	04	04	195	75	-	250	53	(
030	01	1	086	76	LBL	141	42	STO	196	43	RCL	251	43	RCL
031	01	1	087	22	INV	142	03	03	197	03	03	252	20	20
032	42	STO	088	43	RCL	143	43	RCL	198	95	=	253	75	-
033	25	25	089	05	05	144	25	25	199	42	STO	254	43	RCL
034	43	RCL	090	42	STO	145	32	X⇌T	200	09	09	255	11	11
035	23	23	091	01	01	146	01	1	201	53	(	256	54	)
036	65	×	092	01	1	147	06	6	202	43	RCL	257	55	÷
037	05	5	093	02	2	148	77	GE	203	00	00	258	53	(
038	85	+	094	42	STO	149	24	CE	204	75	-	259	43	RCL
039	43	RCL	095	25	25	150	43	RCL	205	43	RCL	260	10	10
040	06	06	096	00	0	151	20	20	206	09	09	261	75	-
041	95	=	097	42	STO	152	55	÷	207	54	)	262	53	(
042	42	STO	098	22	22	153	43	RCL	208	55	÷	263	43	RCL
043	21	21	099	76	LBL	154	10	10	209	53	(	264	11	11
044	43	RCL	100	24	CE	155	95	=	210	53	(	265	55	÷
045	05	05	101	43	RCL	156	42	STO	211	43	RCL	266	43	RCL
046	32	X⇌T	102	01	01	157	24	24	212	00	00	267	22	22
047	43	RCL	103	75	-	158	42	STO	213	55	÷	268	54	)
048	21	21	104	43	RCL	159	23	23	214	43	RCL	269	54	)
049	77	GE	105	23	23	160	00	0	215	09	09	270	54	)
050	22	INV	106	95	=	161	32	X⇌T	216	54	)	271	95	=
051	43	RCL	107	42	STO	162	43	RCL	217	23	LNX	272	42	STO
052	05	05	108	02	02	163	11	11	218	54	)	273	23	23
053	42	STO	109	43	RCL	164	67	EQ	219	95	=	274	61	GTO
054	01	01	110	03	03	165	32	X⇌T	220	42	STO	275	32	X⇌T
055	43	RCL												

User instructions and example for TI version **Table VI**

Step	Value	Example	Key
1.	Store input data:		
	Steam inlet rate, lb/h	9,439	**STO 00**
	Noncondensable rate, lb/h	22,461	**STO 01**
	Molecular wt., noncond., lb/lb mole	35.05	**STO 02**
	Specific heat, inerts, Btu/(lb) (°F)	0.22	**STO 03**
	Operating pressure (abs.), psia	13.97	**STO 04**
	Inlet gas temperature, °F	176	**STO 05**
	Outlet gas temperature, °F	104	**STO 06**
	Coolant inlet temperature, °F	95	**STO 07**
	Coolant outlet temperature, °F	110	**STO 08**
	Pressure drop of vapor, psi	0.25	**STO 09**
2.	Enter program A, sides 1 and 2		
3.	Program performs calculations and prints out the results:		Press **A**
	Saturation temperature, °F	172.228141	
	Q (total), Btu/h	9463302.317	
	Steam rate out, lb/h	976.2570444	
	Steam condensed, lb/h	8462.742956	
	Q (gas cool) incl. desuperheat, Btu/h	483665.5259	
	Q (condensed), Btu/h	8584213.871	
	Q (liquid subcool.), Btu/h	395422.9201	
	Q (desuperheat), Btu/h	34659.49885	
4.	Clear program A and enter program B, sides 1 and 2.		**2nd CP**
5.	Program performs calculations and prints out the results:		Press **A**
	Overall weighted MTD, °F	37.59845717	
	Wtd. MTD saturation zone, °F	37.54995388	
	Wtd. MTD unsaturated zone, °F	57.96768663	
	Saturation temperature, °F	172.228141	

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A new way to rate an existing heat exchanger

With this program, you can quickly determine what will be the unknown temperatures, log-mean temperature-difference correction factor, and heat load for any job that an exchanger may be required to do.

Rogério G. Herkenhoff, Petróleo Brasileiro S.A.

☐ Prediction of the thermal performance of an existing multipass exchanger is usually carried out by an iterative procedure in the following way:

1. Compute the overall heat-transfer coefficient, based on the most recent information about fluid temperatures. (In the first trial, using an arbitrary value may be advantageous.)
2. Calculate the unknown temperatures.
3. If necessary, return to Step 1.

In the second step, one unknown temperature is calculated from a dimensionless group (P), and the other is usually computed via a thermal balance.

The value of P can be obtained graphically [1,2] if the number of shell passes does not exceed two, or by means of a trial-and-error solution involving the calculation of the log-mean temperature-difference (LMTD) correction factor. This time-consuming method can be avoided by using a noniterative general solution.

Developing a general solution

The assumptions are the same as those made for the derivation of the LMTD correction factor [3]. In addition, the number of tube passes must be a multiple of the number of shell passes.

For an exchanger having N shell passes, Bowman [4] developed a general solution for the correction factor:

$$F = \frac{\sqrt{R^2+1}\ln[(1-X)/(1-RX)]}{(R-1)\ln\dfrac{2-X(R+1-\sqrt{R^2+1})}{2-X(R+1+\sqrt{R^2+1})}} \quad (1)$$

where:

$$X = \frac{1-\left(\dfrac{1-RP}{1-P}\right)^{1/N}}{R-\left(\dfrac{1-RP}{1-P}\right)^{1/N}} \quad (2)$$

$$R = \frac{T_1-T_2}{t_2-t_1} = \frac{wc}{WC} \quad (3)$$

$$P = \frac{t_2-t_1}{T_1-t_1} \quad (4)$$

From the original definition:

$$F = \frac{(UA/wc)_{cc}}{(UA/wc)} = \frac{\ln[(1-P)/(1-RP)]}{(R-1)(UA/wc)}$$

Substituting F in Eq. (1):

$$\frac{\ln[(1-P)/(1-RP)]}{(UA/wc)} = \frac{\sqrt{R^2+1}\ln[(1-X)/(1-RX)]}{\ln\dfrac{2-X(R+1-\sqrt{R^2+1})}{2-X(R+1+\sqrt{R^2+1})}} \quad (5)$$

From Eq. (2), it is possible to prove that:

$$\ln[(1-P)/(1-RP)] = N\ln[(1-X)/(1-RX)]$$

Substituting in Eq. (5), and rearranging:

$$X = \frac{2E-2}{(R+1+\sqrt{R^2+1})E-(R+1-\sqrt{R^2+1})} \quad (6)$$

where:

$$E = e^{(UA/wc)\sqrt{R^2+1}/N}$$

From Eq. (2):

$$P = \frac{1-\left(\dfrac{1-RX}{1-X}\right)^{N}}{R-\left(\dfrac{1-RX}{1-X}\right)^{N}} \quad \text{when } (R \neq 1) \quad (7)$$

When $R = 1$, part of the equation becomes indeterminate, but Eq. (6) is still valid. However, Eq. (7) must be replaced by:

$$P = \frac{NX}{NX-X+1} \quad \text{when } (R = 1) \quad (7a)$$

Originally published March 23, 1981.

Program to rate an existing exchanger **Table I**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLa	21 16 11	039	STOI	35 46	077	SPC	16-11	115	P⇄S	16-51	153	RCL8	36 08	191	STOA	35 11
002	STOB	35 12	040	GSB1	23 01	078	2	02	116	GSB9	23 09	154	×	-35	192	RCLE	36 15
003	X⇄Y	-41	041	*LBL1	21 01	079	GSB0	23 00	117	RCLi	36 45	155	RCLC	36 13	193	*LBL2	21 02
004	STOD	35 14	042	GSB5	23 05	080	*LBL2	21 02	118	-	-45	156	÷	-24	194	-	-45
005	RTN	24	043	RCLE	36 15	081	1	01	119	×	-35	157	RCLB	36 12	195	RCLA	36 11
006	*LBLb	21 16 12	044	×	-35	082	P⇄S	16-51	120	RCLi	36 45	158	÷	-24	196	*LBL6	21 06
007	P⇄S	16-51	045	STO0	35 00	083	GSB4	23 04	121	+	-55	159	e^x	33	197	1	01
008	GSBc	23 16 13	046	RCLi	36 45	084	P⇄S	16-51	122	GSB9	23 09	160	STO0	35 00	198	-	-45
009	P⇄S	16-51	047	×	-35	085	GTO1	22 01	123	STOi	35 45	161	RCL9	36 09	199	÷	-24
010	RTN	24	048	RCLi	36 45	086	*LBL7	21 07	124	GTO7	22 07	162	×	-35	200	RTN	24
011	*LBLc	21 16 13	049	-	-45	087	PRTX	-14	125	*LBL5	21 05	163	RCL7	36 07	201	*LBL9	21 09
012	STO3	35 03	050	GSB9	23 09	088	*LBL1	21 01	126	GSB8	23 08	164	-	-45	202	DSZI	16 25 46
013	R↓	-31	051	P⇄S	16-51	089	RTN	24	127	STOC	35 13	165	2	02	203	RTN	24
014	STO4	35 04	052	RCLi	36 45	090	RCLA	36 11	128	P⇄S	16-51	166	RCL0	36 00	204	ISZI	16 26 46
015	R↓	-31	053	P⇄S	16-51	091	1/X	52	129	GSB8	23 08	167	×	-35	205	ISZI	16 26 46
016	STO5	35 05	054	RCLA	36 11	092	GSB3	23 03	130	P⇄S	16-51	168	2	02	206	RTN	24
017	RTN	24	055	ST+0	35-55 00	093	1/X	52	131	÷	-24	169	-	-45	207	*LBL8	21 08
018	*LBLd	21 16 14	056	×	-35	094	LN	32	132	1	01	170	÷	-24	208	RCL1	36 01
019	X⇄Y	-41	057	+	-55	095	RCLE	36 15	133	STO7	35 07	171	GSB3	23 03	209	RCL2	36 02
020	P⇄S	16-51	058	RCL0	36 00	096	GSB6	23 06	134	STO9	35 09	172	RCLB	36 12	210	+	-55
021	GSBe	23 16 15	059	GSB6	23 06	097	RCLD	36 14	135	X⇄Y	-41	173	Y^x	31	211	2	02
022	P⇄S	16-51	060	STOi	35 45	098	÷	-24	136	X≠Y?	16-32	174	GSB3	23 03	212	÷	-24
023	X⇄Y	-41	061	P⇄S	16-51	099	RCL8	36 08	137	GTO1	22 01	175	1/X	52	213	RCL3	36 03
024	RTN	24	062	GTO7	22 07	100	÷	-24	138	EEX	-23	176	STOA	35 11	214	×	-35
025	*LBLe	21 16 15	063	*LBLC	21 13	101	RCLC	36 13	139	5	05	177	RTN	24	215	RCL4	36 04
026	STO2	35 02	064	SPC	16-11	102	×	-35	140	CHS	-22	178	*LBL0	21 00	216	+	-55
027	X⇄Y	-41	065	GSB1	23 01	103	R/S	51	141	+	-55	179	STOI	35 46	217	STO6	35 06
028	STO1	35 01	066	GTO2	22 02	104	GSB8	23 08	142	*LBL1	21 01	180	GSB5	23 05	218	RCL5	36 05
029	RTN	24	067	*LBLD	21 14	105	RCL2	36 02	143	STOE	35 15	181	P⇄S	16-51	219	×	-35
030	*LBLA	21 11	068	SPC	16-11	106	RCL1	36 01	144	ST+7	35-55 07	182	RCLi	36 45	220	RTN	24
031	STO8	35 08	069	1	01	107	-	-45	145	ST+9	35-55 09	183	P⇄S	16-51	221	R/S	51
032	P⇄S	16-51	070	P⇄S	16-51	108	×	-35	146	X^2	53	184	×	-35			
033	STO8	35 08	071	GSB0	23 00	109	RTN	24	147	+	-55	185	RCLi	36 45			
034	P⇄S	16-51	072	P⇄S	16-51	110	*LBL4	21 04	148	√X	54	186	GSB2	23 02			
035	RTN	24	073	*LBL1	21 01	111	STOI	35 46	149	ST-7	35-45 07	187	GSB3	23 03			
036	*LBLB	21 12	074	2	02	112	GSB5	23 05	150	ST+9	35-55 09	188	STOi	35 45			
037	SPC	16-11	075	GTO4	22 04	113	P⇄S	16-51	151	RCLD	36 14	189	GTO7	22 07			
038	2	02	076	*LBLE	21 15	114	RCLi	36 45	152	×	-35	190	*LBL3	21 03			

User's instructions **Table II**

Necessary input (in any order):

1 – $A \uparrow N$	f [a]
2 – $W \uparrow \beta \uparrow \alpha$ (hot fluid)	f [b]
3 – $w \uparrow \beta \uparrow \alpha$ (cold fluid)	f [c]
4 – $T_1 \uparrow T_2$	f [d]
5 – $t_1 \uparrow t_2$	f [e]
6 – U	[A]
Output:	
1 – To print t_1 and T_1	[B]
2 – To print t_2 and T_2	[C]
3 – To print T_1 and t_2	[D]
4 – To print t_1 and T_2	[E]
5 – After pressing B, C, D or E:	
(a) To display F	[R/S]
(b) To display q	[R/S]

Registers:

0	1	2	3	4	5	6	7	8	9
Used	t_1	t_2	α_c	β_c	w	c	Used	U	Used
S0	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**
Used	T_2	T_1	α_h	β_h	W	C	Used	U	Used

A	B	C	D	E	I
Used	N	wc or WC	A	R	Used

where: $c = \beta_c + \alpha_c t_m$

$C = \beta_h + \alpha_h T_m$

When the cold fluid is isothermally vaporized ($R = \infty$), or when in Eq. (4) only one temperature is known, the definitions of R and P [Eq. (3) and (4)] may be changed to:

$$R = \frac{t_2 - t_1}{T_1 - T_2} = \frac{WC}{wc} \tag{3a}$$

$$P = \frac{T_1 - T_2}{T_1 - t_1} \tag{4a}$$

In this case, in Eq. (6), E must be replaced by:

$$E = e^{(UA/WC)\sqrt{R^2+1}/N}$$

Program description

The HP-97/67/41-C program calculates any combination of two terminal temperatures in an existing multipass exchanger, except if both refer to the same fluid.

The specific heats are calculated as a linear function of the arithmetic mean temperatures of the fluids, using the last temperatures stored. Thus, unless the desired temperatures had been preliminarily stored, or the specific heats had been considered to be constants ($\alpha = 0$), the temperatures will not be precisely calculated.

So, an iterative procedure must be used to yield a consistent result. The desired calculation is repeated (by pressing B, C, D or E) until the calculated temperatures remain approximately constant. An initial estimate of the desired temperatures may be stored to avoid using the remaining values of any previous operation and to improve the convergence.

Also, the overall heat-transfer coefficient is often seriously affected by the variation of the physical properties of the fluids and cannot be precisely evaluated without knowledge of both inlet and outlet fluid temperatures. Therefore, the iterative procedure must usually include the replacement of the previous estimate of the overall coefficient with a new one, computed for the latest temperature conditions.

After the convergence, the program can calculate the LMTD correction factor and the heat load, based on the cold-fluid conditions.

Any system of units may be used, as long as UA/wc remains dimensionless.

The program can also accommodate a pure counterflow exchanger, assuming a number of shell passes sufficiently large to make the LMTD correction factor equal to 1.

When $R = 1$, the program assumes $R = 1.00001$ to permit the solution without using Eq. (7a).

The second unknown temperature is calculated from a second value of P, which is evaluated by using the first calculated temperature to compute the specific heat.

Rating an exchanger for heating crude oil

It is desired to heat 700,000 lb/h of a 36.4° API gravity crude ($k = 11.5$) at 433°F, using 400,000 lb/h of a 38° API gravity oil ($k = 12.1$) at 556°F. Available for this service is a 3:6 exchanger having a heat-transfer surface area of 15,000 ft^2. Assuming a total dirt factor of 0.005, and that the individual heat-transfer coefficients may be estimated by the following equations, what will the outlet temperatures be?

$$h_c = 25 + 0.35\, t_m \quad \text{and} \quad h_h = 160 + 0.30\, T_m$$

Using the equation presented in Ref. 2, p. 149:

$$\beta_c = 0.4142$$
$$\alpha_c = 0.0005474$$
$$\beta_h = 0.4306$$
$$\alpha_h = 0.0005682$$

In the first trial, let us assume that $U = 50$, $t_2 = t_1$, and $T_2 = T_1$.

Preliminary input:

1—15,000↑3 f [a]
2—400,000↑.4306↑.0005682 f [b]
3—700,000↑.4142↑.0005474 f [c]
4—556↑ f [d]
5—433↑ f [e]

1st trial:

1—50 [A]
2—(Compute t_2 and T_2) [C] ($t_2 = 496.01$, $T_2 = 459.29$)

2nd trial:

1—Compute the overall coefficient ($U = 73.89$)
2—73.89 [A]
3—Compute t_2 and T_2 [C] ($t_2 = 498.77$, $T_2 = 448.98$)

3rd trial:

1—Compute the overall coefficient ($U = 73.88$)
2—73.88 [A]
3—Compute t_2 and T_2 [C] ($t_2 = 498.53$, $T_2 = 448.83$)

4th trial:

1—Compute the overall coefficient ($U = 73.87$)
2—73.87 [A]
3—Compute t_2 and T_2 [C] ($t_2 = 498.53$, $T_2 = 448.83$)
4—Compute F [R/S] ($F = 0.85792$)
5—Compute q [R/S] ($q = 3.06972 \times 10^7$)

Nomenclature

- A Heat-transfer surface area
- c Cold-fluid specific heat
- C Hot-fluid specific heat
- E Dimensionless group
- F LMTD correction factor
- h Individual heat-transfer coefficient
- k Characterization factor
- N Total number of shell passes
- P Dimensionless group
- q Heat load
- R Dimensionless group
- R_d Fouling factor
- t Cold-fluid temperature
- T Hot-fluid temperature
- U Overall heat-transfer coefficient
- w Cold-fluid mass flowrate
- W Hot-fluid mass flowrate
- X Dimensionless group
- α Angular coefficient for specific-heat calculation
- β Linear coefficient for specific-heat calculation

Subscripts

- c Cold fluid
- cc Countercurrent
- h Hot fluid
- m Arithmetic mean
- 1 Inlet
- 2 Outlet

For TI-58/59 users

The TI programs closely follow the HP version. However, program A (see Table III listing) supplies output 1 and 2 of Table II. (i.e., output 1 is inlet temperatures, and output 2 is outlet temperatures). Program B (listing in Table IV) offers output 3 and 4. Table V provides user instructions.

Listing for TI version—program A **Table III**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	012	42	STO	024	65	×
001	11	A	013	25	25	025	43	RCL
002	42	STO	014	71	SBR	026	24	24
003	08	08	015	22	INV	027	95	=
004	42	STO	016	71	SBR	028	42	STO
005	18	18	017	23	LNX	029	00	00
006	01	1	018	76	LBL	030	65	×
007	32	X:T	019	22	INV	031	73	RC*
008	91	R/S	020	71	SBR	032	25	25
009	76	LBL	021	24	CE	033	75	−
010	12	B	022	43	RCL	034	73	RC*
011	02	2	023	20	20	035	25	25

(Continued) Table III

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
036	95	=	100	61	GTO	164	25	25	228	65	+	292	43	RCL
037	42	STO	101	34	√X	165	67	EQ	229	01	1	293	24	24
038	40	40	102	76	LBL	166	44	SUM	230	95	=	294	95	=
039	01	1	103	33	X²	167	02	2	231	34	√X	295	55	÷
040	22	INV	104	02	2	168	42	STO	232	22	INV	296	53	(
041	44	SUM	105	42	STO	169	25	25	233	44	SUM	297	43	RCL
042	25	25	106	25	25	170	76	LBL	234	07	07	298	20	20
043	43	RCL	107	61	GTO	171	44	SUM	235	44	SUM	299	75	-
044	25	25	108	42	STO	172	43	RCL	236	09	09	300	01	1
045	67	EQ	109	76	LBL	173	43	43	237	65	×	301	54	)
046	25	CLR	110	34	√X	174	72	ST*	238	43	RCL	302	95	=
047	02	2	111	71	SBR	175	25	25	239	23	23	303	35	1/X
048	42	STO	112	23	LNX	176	99	PRT	240	65	×	304	42	STO
049	25	25	113	01	1	177	61	GTO	241	43	RCL	305	20	20
050	76	LBL	114	42	STO	178	45	Y^X	242	08	08	306	92	RTN
051	25	CLR	115	25	25	179	76	LBL	243	55	÷	307	76	LBL
052	43	RCL	116	71	SBR	180	24	CE	244	43	RCL	308	52	EE
053	20	20	117	42	STO	181	71	SBR	245	22	22	309	53	(
054	44	SUM	118	76	LBL	182	52	EE	246	55	÷	310	43	RCL
055	00	00	119	42	STO	183	43	RCL	247	43	RCL	311	01	01
056	71	SBR	120	71	SBR	184	44	44	248	21	21	312	85	+
057	23	LNX	121	24	CE	185	42	STO	249	95	=	313	43	RCL
058	73	RC*	122	71	SBR	186	22	22	250	22	INV	314	02	02
059	25	25	123	23	LNX	187	71	SBR	251	23	LNX	315	54	)
060	65	×	124	73	RC*	188	23	LNX	252	42	STO	316	55	÷
061	43	RCL	125	25	25	189	71	SBR	253	00	00	317	02	2
062	20	20	126	42	STO	190	52	EE	254	65	×	318	65	×
063	85	+	127	42	42	191	71	SBR	255	43	RCL	319	43	RCL
064	43	RCL	128	71	SBR	192	23	LNX	256	09	09	320	03	03
065	40	40	129	23	LNX	193	43	RCL	257	75	-	321	85	+
066	95	=	130	01	1	194	22	22	258	43	RCL	322	43	RCL
067	42	STO	131	22	INV	195	55	÷	259	07	07	323	04	04
068	41	41	132	44	SUM	196	43	RCL	260	95	=	324	95	=
069	71	SBR	133	25	25	197	44	44	261	55	÷	325	42	STO
070	23	LNX	134	43	RCL	198	95	=	262	53	(	326	06	06
071	43	RCL	135	25	25	199	42	STO	263	02	2	327	65	×
072	41	41	136	67	EQ	200	45	45	264	65	×	328	43	RCL
073	55	÷	137	43	RCL	201	01	1	265	43	RCL	329	05	05
074	53	(	138	02	2	202	42	STO	266	00	00	330	95	=
075	43	RCL	139	42	STO	203	07	07	267	75	-	331	42	STO
076	00	00	140	25	25	204	42	STO	268	02	2	332	44	44
077	75	-	141	76	LBL	205	09	09	269	54	)	333	92	RTN
078	01	1	142	43	RCL	206	43	RCL	270	95	=	334	76	LBL
079	54	)	143	53	(	207	45	45	271	42	STO	335	23	LNX
080	95	=	144	43	RCL	208	22	INV	272	20	20	336	00	0
081	72	ST*	145	42	42	209	67	EQ	273	75	-	337	42	STO
082	25	25	146	75	-	210	53	(	274	43	RCL	338	49	49
083	76	LBL	147	73	RC*	211	01	1	275	24	24	339	76	LBL
084	55	÷	148	25	25	212	52	EE	276	95	=	340	61	GTO
085	73	RC*	149	54	)	213	94	+/-	277	55	÷	341	73	RC*
086	25	25	150	65	×	214	05	5	278	53	(	342	49	49
087	99	PRT	151	43	RCL	215	44	SUM	279	43	RCL	343	32	X⇌T
088	76	LBL	152	20	20	216	45	45	280	20	20	344	01	1
089	45	Y^X	153	85	+	217	76	LBL	281	75	-	345	00	0
090	87	IFF	154	73	RC*	218	53	(	282	01	1	346	44	SUM
091	01	01	155	25	25	219	43	RCL	283	54	)	347	49	49
092	32	X⇌T	156	95	=	220	45	45	284	95	=	348	73	RC*
093	86	STF	157	42	STO	221	42	STO	285	45	Y^X	349	49	49
094	01	01	158	43	43	222	24	24	286	43	RCL	350	32	X⇌T
095	92	RTN	159	01	1	223	44	SUM	287	21	21	351	72	ST*
096	76	LBL	160	22	INV	224	07	07	288	95	=	352	49	49
097	13	C	161	44	SUM	225	44	SUM	289	42	STO	353	01	1
098	71	SBR	162	25	25	226	09	09	290	20	20	354	00	0
099	33	X²	163	43	RCL	227	33	X²	291	75	-	355	22	INV

(Continued) Table III

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
356	44	SUM	376	32	X:T	396	75	-	416	43	RCL	436	42	STO
357	49	49	377	92	RTN	397	01	1	417	08	08	437	06	06
358	32	X:T	378	76	LBL	398	54	)	418	95	=	438	71	SBR
359	72	ST*	379	32	X:T	399	95	=	419	99	PRT	439	23	LNX
360	49	49	380	22	INV	400	35	1/X	420	53	(	440	43	RCL
361	01	1	381	86	STF	401	23	LNX	421	43	RCL	441	06	06
362	44	SUM	382	01	01	402	65	×	422	01	01	442	65	×
363	49	49	383	43	RCL	403	43	RCL	423	85	+	443	43	RCL
364	01	1	384	20	20	404	22	22	424	43	RCL	444	05	05
365	00	0	385	35	1/X	405	55	÷	425	02	02	445	65	×
366	32	X:T	386	42	STO	406	53	(	426	54	)	446	53	(
367	43	RCL	387	20	20	407	43	RCL	427	55	÷	447	43	RCL
368	49	49	388	75	-	408	24	24	428	02	2	448	02	02
369	67	EQ	389	43	RCL	409	75	-	429	65	×	449	75	-
370	65	×	390	24	24	410	01	1	430	43	RCL	450	43	RCL
371	61	GTO	391	95	=	411	54	)	431	03	03	451	01	01
372	61	GTO	392	55	÷	412	55	÷	432	85	+	452	54	)
373	76	LBL	393	53	(	413	43	RCL	433	43	RCL	453	95	=
374	65	×	394	43	RCL	414	23	23	434	04	04	454	99	PRT
375	01	1	395	20	20	415	55	÷	435	95	=	455	91	R/S

Listing for VI version—program B **Table IV**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	036	42	STO	072	43	RCL	108	76	LBL	144	43	RCL
001	11	A	037	25	25	073	25	25	109	44	SUM	145	45	45
002	42	STO	038	61	GTO	074	67	EQ	110	43	RCL	146	22	INV
003	08	08	039	42	STO	075	43	RCL	111	43	43	147	67	EQ
004	42	STO	040	76	LBL	076	02	2	112	72	ST*	148	53	(
005	18	18	041	15	E	077	42	STO	113	25	25	149	01	1
006	01	1	042	02	2	078	25	25	114	99	PRT	150	52	EE
007	32	X:T	043	42	STO	079	76	LBL	115	61	GTO	151	94	+/-
008	91	R/S	044	25	25	080	43	RCL	116	45	Yˣ	152	05	5
009	76	LBL	045	71	SBR	081	53	(	117	76	LBL	153	44	SUM
010	55	÷	046	35	1/X	082	43	RCL	118	24	CE	154	45	45
011	73	RC*	047	76	LBL	083	42	42	119	71	SBR	155	76	LBL
012	25	25	048	34	ΓX	084	75	-	120	52	EE	156	53	(
013	99	PRT	049	71	SBR	085	73	RC*	121	43	RCL	157	43	RCL
014	76	LBL	050	23	LNX	086	25	25	122	44	44	158	45	45
015	45	Yˣ	051	01	1	087	54	)	123	42	STO	159	42	STO
016	87	IFF	052	42	STO	088	65	×	124	22	22	160	24	24
017	01	01	053	25	25	089	43	RCL	125	71	SBR	161	44	SUM
018	32	X:T	054	71	SBR	090	20	20	126	23	LNX	162	07	07
019	86	STF	055	42	STO	091	85	+	127	71	SBR	163	44	SUM
020	01	01	056	76	LBL	092	73	RC*	128	52	EE	164	09	09
021	92	RTN	057	42	STO	093	25	25	129	71	SBR	165	33	X²
022	76	LBL	058	71	SBR	094	95	=	130	23	LNX	166	85	+
023	14	D	059	24	CE	095	42	STO	131	43	RCL	167	01	1
024	01	1	060	71	SBR	096	43	43	132	22	22	168	95	=
025	42	STO	061	23	LNX	097	01	1	133	55	÷	169	34	ΓX
026	25	25	062	73	RC*	098	22	INV	134	43	RCL	170	22	INV
027	71	SBR	063	25	25	099	44	SUM	135	44	44	171	44	SUM
028	23	LNX	064	42	STO	100	25	25	136	95	=	172	07	07
029	71	SBR	065	42	42	101	43	RCL	137	42	STO	173	44	SUM
030	35	1/X	066	71	SBR	102	25	25	138	45	45	174	09	09
031	71	SBR	067	23	LNX	103	67	EQ	139	01	1	175	65	×
032	23	LNX	068	01	1	104	44	SUM	140	42	STO	176	43	RCL
033	76	LBL	069	22	INV	105	02	2	141	07	07	177	23	23
034	33	X²	070	44	SUM	106	42	STO	142	42	STO	178	65	×
035	02	2	071	25	25	107	25	25	143	09	09	179	43	RCL

(Continued) Table IV

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
180	08	08	233	55	÷	286	42	STO	339	32	X:T	392	43	RCL
181	55	÷	234	53	(	287	25	25	340	72	ST*	393	22	22
182	43	RCL	235	43	RCL	288	76	LBL	341	49	49	394	55	÷
183	22	22	236	20	20	289	54	)	342	01	1	395	53	(
184	55	÷	237	75	-	290	43	RCL	343	00	0	396	43	RCL
185	43	RCL	238	01	1	291	48	48	344	22	INV	397	24	24
186	21	21	239	54	)	292	72	ST*	345	44	SUM	398	75	-
187	95	=	240	95	=	293	25	25	346	49	49	399	01	1
188	22	INV	241	35	1/X	294	61	GTO	347	32	X:T	400	54	)
189	23	LNX	242	42	STO	295	55	÷	348	72	ST*	401	55	÷
190	42	STO	243	20	20	296	76	LBL	349	49	49	402	43	RCL
191	00	00	244	92	RTN	297	52	EE	350	01	1	403	23	23
192	65	×	245	76	LBL	298	53	(	351	44	SUM	404	55	÷
193	43	RCL	246	35	1/X	299	43	RCL	352	49	49	405	43	RCL
194	09	09	247	71	SBR	300	01	01	353	01	1	406	08	08
195	75	-	248	24	CE	301	85	+	354	00	0	407	95	=
196	43	RCL	249	71	SBR	302	43	RCL	355	32	X:T	408	99	PRT
197	07	07	250	23	LNX	303	02	02	356	43	RCL	409	53	(
198	95	=	251	43	RCL	304	54	)	357	49	49	410	43	RCL
199	55	÷	252	20	20	305	55	÷	358	67	EQ	411	01	01
200	53	(	253	65	×	306	02	2	359	65	×	412	85	+
201	02	2	254	73	RC*	307	65	×	360	61	GTO	413	43	RCL
202	65	×	255	25	25	308	43	RCL	361	61	GTO	414	02	02
203	43	RCL	256	95	=	309	03	03	362	76	LBL	415	54	)
204	00	00	257	42	STO	310	85	+	363	65	×	416	55	÷
205	75	-	258	47	47	311	43	RCL	364	01	1	417	02	2
206	02	2	259	71	SBR	312	04	04	365	32	X:T	418	65	×
207	54	)	260	23	LNX	313	95	=	366	92	RTN	419	43	RCL
208	95	=	261	43	RCL	314	42	STO	367	76	LBL	420	03	03
209	42	STO	262	47	47	315	06	06	368	32	X:T	421	85	+
210	20	20	263	75	-	316	65	×	369	22	INV	422	43	RCL
211	75	-	264	73	RC*	317	43	RCL	370	86	STF	423	04	04
212	43	RCL	265	25	25	318	05	05	371	01	01	424	95	=
213	24	24	266	95	=	319	95	=	372	43	RCL	425	42	STO
214	95	=	267	55	÷	320	42	STO	373	20	20	426	06	06
215	55	÷	268	53	(	321	44	44	374	35	1/X	427	71	SBR
216	53	(	269	43	RCL	322	92	RTN	375	42	STO	428	23	LNX
217	43	RCL	270	20	20	323	76	LBL	376	20	20	429	43	RCL
218	20	20	271	75	-	324	23	LNX	377	75	-	430	06	06
219	75	-	272	01	1	325	00	0	378	43	RCL	431	65	×
220	01	1	273	54	)	326	42	STO	379	24	24	432	43	RCL
221	54	)	274	95	=	327	49	49	380	95	=	433	05	05
222	95	=	275	42	STO	328	76	LBL	381	55	÷	434	65	×
223	45	Y^X	276	48	48	329	61	GTO	382	53	(	435	53	(
224	43	RCL	277	01	1	330	73	RC*	383	43	RCL	436	43	RCL
225	21	21	278	22	INV	331	49	49	384	20	20	437	02	02
226	95	=	279	44	SUM	332	32	X:T	385	75	-	438	75	-
227	42	STO	280	25	25	333	01	1	386	01	1	439	43	RCL
228	20	20	281	43	RCL	334	00	0	387	54	)	440	01	01
229	75	-	282	25	25	335	44	SUM	388	95	=	441	54	)
230	43	RCL	283	67	EQ	336	49	49	389	35	1/X	442	95	=
231	24	24	284	54	)	337	73	RC*	390	23	LNX	443	99	PRT
232	95	=	285	02	2	338	49	49	391	65	×	444	91	R/S

User instructions for TI version **Table V**

Two separate programs are given. They are run in similar manner.

For both programs data are entered as follows:

A, heat-transfer surface area	**STO 23**
N, number of passes	**STO 21**
Hot side	
W, mass flowrate	**STO 15**
α factor	**STO 13**
β factor	**STO 14**
T_1, temperature in	**STO 12**
T_2, temperature out	**STO 11**
Cold side	
w, mass flowrate	**STO 05**
α factor	**STO 03**
β factor	**STO 04**
t_1, temperature in	**STO 01**
t_2, temperature out	**STO 02**

Enter estimate of overall heat-transfer coefficient *U*, then press key **A**

With the program A:

Key **B** gives inlet temperatures, cold side (t_1) and hot side (T_1)
Key **C** gives outlet temperatures, cold side (t_2) and hot side (T_2)

With program B:

Key **D** gives hot side inlet (T_1) and cold side outlet (t_2) temperatures
Key **E** gives cold side inlet (t_1) and hot side outlet (T_2) temperatures

Calculation will take a few minutes. In all cases, programs also give LMTD correction factor *F*, and heat load *q*.

With further estimate of overall heat-transfer coefficient, key **A**, additional calculations of the same two temperatures are made until satisfactory convergence is obtained.

(Note: Any consistent set of units may be used as long as *UA/wc* remains dimensionless.)

All output are printed in the order indicated in the explanation (i.e., temperatures, LMTD correction factor *F*, and heat load *q*.).

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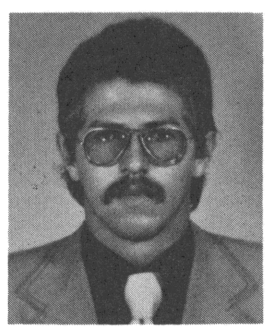

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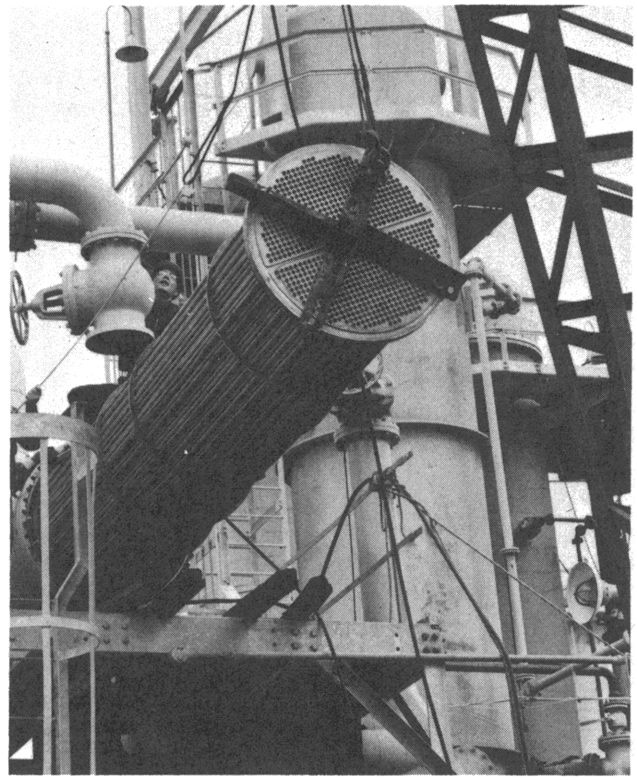
Calculating the corrected LMTD in shell-and-tube heat exchangers



The programs described here, one for the Hewlett-Packard system and one for the Texas Instruments system, will allow the engineer to calculate the corrected logarithmic mean temperature-difference for shell-and-tube heat exchangers in series.

*W. Wayne **Blackwell**, Ford, Bacon & Davis, Texas Inc., and **Larry Haydu**, Kennecott Corp.*

☐ Heat transfer is more efficient when there is countercurrent flow rather than cocurrent flow. When multipass shell-and-tube exchangers are used in series, the flow more closely approximates countercurrent when a lot of shells are used. But this means greater cost. So it is desirable to use the minimum number of shells that will achieve an acceptable level of efficiency.

The programs described here will determine that minimum number of shells, and will calculate a corrected mean temperature-difference for the system chosen. This eliminates the need for laborious calculations with charts and graphs that are normally used in such designs.

Heat-exchanger design

The thermal design of heat-exchange equipment often requires the calculation of the logarithmic mean temperature-difference (LMTD). This is defined by the following equation:

$$\text{LMTD} = \frac{\Delta t_1 - \Delta t_2}{\ln \dfrac{\Delta t_1}{\Delta t_2}}$$

Where, for countercurrent flow:
Δt_1 = the larger terminal difference, $T_1 - t_2$, and
Δt_2 = the smaller terminal difference, $T_2 - t_1$.

For cocurrent flow,
$\Delta t_1 = T_1 - t_1$, and
$\Delta t_2 = T_2 - t_2$.

Temperatures:
T_1 = hot-fluid inlet temperature, °F,
T_2 = hot-fluid exit temperature, °F,
t_1 = cold-fluid inlet temperature, °F,
t_2 = cold-fluid exit temperature, °F.

Fig. 1 shows a typical temperature profile of two fluids in true countercurrent flow through a 1-1 exchanger (one shell pass, one tube pass).

The 1-1 exchanger is very simple but has its limitations. In the majority of industrial operations, higher velocities, shorter tubes, and a more economical exchanger can be found using multipass design. In a multipass exchanger such as shown in Fig. 2, the flow is part countercurrent and part cocurrent. As a result, the mean temperature difference lies somewhere between the countercurrent and cocurrent LMTDs.

In this situation, a correction factor, F, is defined so that, when it is multiplied by the LMTD, the product is the corrected mean temperature-difference (CMTD).

$$\text{CMTD} = F \times \text{LMTD}$$

Thus, for pure countercurrent flow, $F = 1$. As more cocurrent flow is introduced, F is reduced and the efficiency of the exchanger drops. The lower limit of prac-

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Hewlett-Packard program listing **Table I**

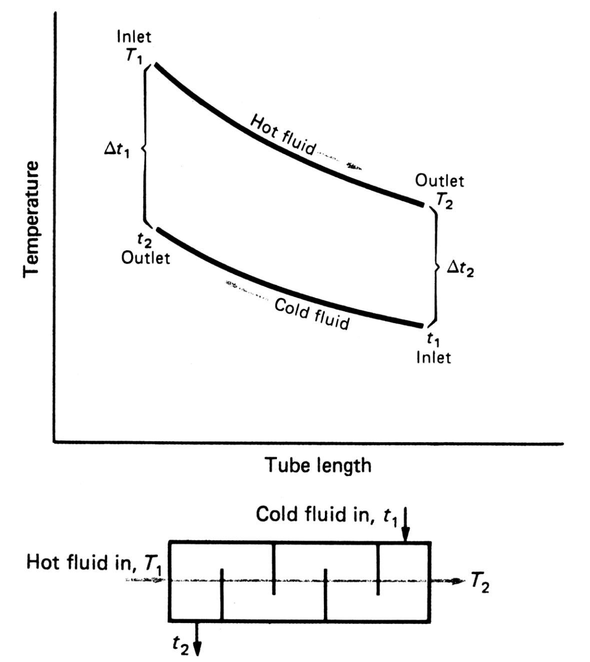
Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	038	RCL1	36 01	075	÷	-24	112	X<0?	16-45	149	GTOB	22 12	186	X⇄Y	-41
002	1	01	039	RCL2	36 02	076	STO9	35 09	113	GTOC	22 13	150	*LBLD	21 14	187	X=Y?	16-33
003	STCI	35 46	040	-	-45	077	2	02	114	1	01	151	RCLI	36 46	188	GTOC	22 13
004	P⇄S	16-51	041	RCL4	36 04	078	X⇄Y	-41	115	X⇄Y	-41	152	RCL5	36 05	189	LN	32
005	.	-62	042	RCL3	36 03	079	÷	-24	116	X=Y?	16-33	153	×	-35	190	P⇄S	16-51
006	8	08	043	-	-45	080	1	01	117	GTOC	22 13	154	CHS	-22	191	STO1	35 01
007	STO2	35 02	044	X=0?	16-43	081	-	-45	118	LN	32	155	RCL5	36 05	192	P⇄S	16-51
008	P⇄S	16-51	045	GTOd	22 16 14	082	RCL6	36 06	119	RCL7	36 07	156	+	-55	193	RCL9	36 09
009	RCL1	36 01	046	÷	-24	083	-	-45	120	×	-35	157	RCLI	36 46	194	RCL7	36 07
010	RCL4	36 04	047	STO6	35 06	084	P⇄S	16-51	121	RCL6	36 06	158	+	-55	195	×	-35
011	-	-45	048	X^2	53	085	STO0	35 00	122	1	01	159	RCL5	36 05	196	1	01
012	ABS	16 31	049	1	01	086	P⇄S	16-51	123	-	-45	160	X⇄Y	-41	197	RCL9	36 09
013	STO5	35 05	050	+	-55	087	RCL7	36 07	124	÷	-24	161	÷	-24	198	-	-45
014	RCL2	36 02	051	√X	54	088	+	-55	125	P⇄S	16-51	162	STO9	35 09	199	÷	-24
015	RCL3	36 03	052	STO7	35 07	089	P⇄S	16-51	126	RCL1	36 01	163	2	02	200	P⇄S	16-51
016	-	-45	053	1	01	090	RCL0	36 00	127	÷	-24	164	X⇄Y	-41	201	RCL1	36 01
017	ABS	16 31	054	RCL6	36 06	091	P⇄S	16-51	128	P⇄S	16-51	165	÷	-24	202	÷	-24
018	STO6	35 06	055	X=Y?	16-33	092	RCL7	36 07	129	*LBLE	21 15	166	1	01	203	P⇄S	16-51
019	-	-45	056	GTOD	22 14	093	-	-45	130	STOD	35 14	167	-	-45	204	GTOE	22 15
020	X=0?	16-43	057	RCL5	36 05	094	X=0?	16-43	131	RCL0	36 00	168	RCL6	36 06	205	*LBLb	21 16 12
021	GTOb	22 16 12	058	×	-35	095	GTOC	22 13	132	X=0?	16-43	169	-	-45	206	RCL5	36 05
022	RCL5	36 05	059	1	01	096	÷	-24	133	GSBc	23 16 13	170	P⇄S	16-51	207	STOB	35 12
023	RCL6	36 06	060	-	-45	097	X<0?	16-45	134	X>Y?	16-34	171	STO0	35 00	208	GTOa	22 16 11
024	÷	-24	061	RCL5	36 05	098	GTOC	22 13	135	GTOC	22 13	172	P⇄S	16-51	209	*LBLd	21 16 14
025	LN	32	062	1	01	099	LN	32	136	RCLI	36 46	173	RCL7	36 07	210	RCLB	36 12
026	÷	-24	063	-	-45	100	P⇄S	16-51	137	STOA	35 11	174	+	-55	211	STOC	35 13
027	*LBLa	21 16 11	064	÷	-24	101	STO1	35 01	138	SPC	16-11	175	P⇄S	16-51	212	1	01
028	STOB	35 12	065	RCLI	36 46	102	P⇄S	16-51	139	PRTX	-14	176	RCL0	36 00	213	GTOE	22 15
029	*LBLB	21 12	066	1/X	52	103	1	01	140	RCLB	36 12	177	P⇄S	16-51	214	*LBLc	21 16 13
030	RCL4	36 04	067	Y^x	31	104	RCL9	36 09	141	PRTX	-14	178	RCL7	36 07	215	R↓	-31
031	RCL3	36 03	068	STO8	35 08	105	-	-45	142	RCLD	36 14	179	-	-45	216	P⇄S	16-51
032	-	-45	069	1	01	106	1	01	143	×	-35	180	X=0?	16-43	217	RCL2	36 02
033	RCL1	36 01	070	X⇄Y	-41	107	RCL9	36 09	144	STOC	35 13	181	GTOC	22 13	218	P⇄S	16-51
034	RCL3	36 03	071	-	-45	108	RCL6	36 06	145	PRTX	-14	182	÷	-24	219	RTN	24
035	-	-45	072	RCL6	36 06	109	×	-35	146	RTN	24	183	X<0?	16-45	220	R/S	51
036	÷	-24	073	RCL8	36 08	110	-	-45	147	*LBLC	21 13	184	GTOC	22 13			
037	STO5	35 05	074	-	-45	111	÷	-24	148	ISZI	16 26 46	185	1	01			

Texas Instruments program listing **Table II**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	022	43	RCL	044	43	RCL	066	42	STO	088	69	OP
001	11	A	023	25	25	045	20	20	067	02	02	089	02	02
002	04	4	024	69	OP	046	69	OP	068	43	RCL	090	69	OP
003	69	OP	025	03	03	047	02	02	069	20	20	091	05	05
004	17	17	026	69	OP	048	69	OP	070	69	OP	092	43	RCL
005	25	CLR	027	05	05	049	05	05	071	02	02	093	24	24
006	69	OP	028	69	OP	050	91	R/S	072	69	OP	094	91	R/S
007	00	00	029	00	00	051	42	STO	073	05	05	095	42	STO
008	43	RCL	030	43	RCL	052	01	01	074	91	R/S	096	04	04
009	16	16	031	18	18	053	99	PRT	075	42	STO	097	99	PRT
010	69	OP	032	69	OP	054	43	RCL	076	03	03	098	53	(
011	02	02	033	01	01	055	21	21	077	99	PRT	099	43	RCL
012	43	RCL	034	43	RCL	056	69	OP	078	76	LBL	100	00	00
013	17	17	035	19	19	057	01	01	079	12	B	101	75	-
014	69	OP	036	69	OP	058	43	RCL	080	69	OP	102	43	RCL
015	03	03	037	02	02	059	19	19	081	00	00	103	01	01
016	69	OP	038	69	OP	060	69	OP	082	43	RCL	104	54	)
017	05	05	039	05	05	061	02	02	083	22	22	105	55	÷
018	43	RCL	040	91	R/S	062	69	OP	084	69	OP	106	53	(
019	25	25	041	42	STO	063	05	05	085	01	01	107	43	RCL
020	69	OP	042	00	00	064	91	R/S	086	43	RCL	108	03	03
021	02	02	043	99	PRT	065	99	PRT	087	23	23	109	75	-

Texas Instruments program listing **Table II (continued)**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
110	43	RCL	176	02	2	242	75	-	308	77	GE	374	03	03	440	31	31
111	02	02	177	85	+	243	01	1	309	18	C'	375	43	RCL	441	69	OP
112	54	)	178	02	2	244	95	=	310	28	LOG	376	27	27	442	02	02
113	95	=	179	34	√X	245	55	÷	311	42	STO	377	69	OP	443	43	RCL
114	42	STO	180	95	=	246	53	(	312	10	10	378	04	04	444	32	32
115	06	06	181	42	STO	247	43	RCL	313	01	1	379	69	OP	445	69	OP
116	53	(	182	10	10	248	07	07	314	75	-	380	05	05	446	03	03
117	43	RCL	183	02	2	249	75	-	315	43	RCL	381	43	RCL	447	69	OP
118	03	03	184	55	÷	250	01	1	316	05	05	382	04	04	448	05	05
119	75	-	185	43	RCL	251	54	)	317	95	=	383	99	PRT	449	43	RCL
120	43	RCL	186	08	08	252	95	=	318	55	÷	384	61	GTO	450	14	14
121	02	02	187	75	-	253	45	Y^X	319	53	(	385	34	√X	451	65	×
122	54	)	188	02	2	254	43	RCL	320	01	1	386	76	LBL	452	43	RCL
123	55	÷	189	75	-	255	04	04	321	75	-	387	16	A'	453	11	11
124	53	(	190	02	2	256	35	1/X	322	43	RCL	388	25	CLR	454	95	=
125	43	RCL	191	34	√X	257	95	=	323	05	05	389	32	X:T	455	99	PRT
126	00	00	192	95	=	258	42	STO	324	65	×	390	43	RCL	456	98	ADV
127	75	-	193	22	INV	259	15	15	325	43	RCL	391	01	01	457	98	ADV
128	43	RCL	194	49	PRD	260	94	+/-	326	06	06	392	75	-	458	98	ADV
129	02	02	195	10	10	261	85	+	327	54	)	393	43	RCL	459	91	R/S
130	54	)	196	25	CLR	262	01	1	328	95	=	394	02	02	460	76	LBL
131	95	=	197	32	X:T	263	95	=	329	28	LOG	395	95	=	461	17	B'
132	42	STO	198	43	RCL	264	55	÷	330	65	×	396	42	STO	462	43	RCL
133	07	07	199	10	10	265	53	(	331	43	RCL	397	12	12	463	12	12
134	43	RCL	200	22	INV	266	43	RCL	332	09	09	398	43	RCL	464	42	STO
135	06	06	201	77	GE	267	06	06	333	55	÷	399	00	00	465	14	14
136	33	X^2	202	18	C'	268	75	-	334	53	(	400	75	-	466	61	GTO
137	85	+	203	28	LOG	269	43	RCL	335	43	RCL	401	43	RCL	467	15	E
138	01	1	204	42	STO	270	15	15	336	06	06	402	03	03	468	76	LBL
139	95	=	205	10	10	271	54	)	337	75	-	403	95	=	469	45	Y^X
140	34	√X	206	43	RCL	272	95	=	338	01	1	404	42	STO	470	69	OP
141	42	STO	207	09	09	273	42	STO	339	54	)	405	13	13	471	00	00
142	09	09	208	65	×	274	05	05	340	95	=	406	75	-	472	43	RCL
143	76	LBL	209	43	RCL	275	35	1/X	341	55	÷	407	43	RCL	473	28	28
144	34	√X	210	08	08	276	65	×	342	43	RCL	408	12	12	474	69	OP
145	01	1	211	55	÷	277	02	2	343	10	10	409	95	=	475	02	02
146	32	X:T	212	53	(	278	75	-	344	95	=	410	67	EQ	476	43	RCL
147	43	RCL	213	01	1	279	01	1	345	42	STO	411	17	B'	477	29	29
148	06	06	214	00	0	280	75	-	346	11	11	412	55	÷	478	69	OP
149	22	INV	215	23	LNX	281	43	RCL	347	76	LBL	413	53	(	479	03	03
150	67	EQ	216	65	×	282	06	06	348	14	D	414	43	RCL	480	69	OP
151	13	C	217	53	(	283	85	+	349	71	SBR	415	13	13	481	05	05
152	43	RCL	218	01	1	284	43	RCL	350	45	Y^X	416	55	÷	482	43	RCL
153	07	07	219	75	-	285	09	09	351	43	RCL	417	43	RCL	483	11	11
154	55	÷	220	43	RCL	286	95	=	352	33	33	418	12	12	484	99	PRT
155	53	(	221	08	08	287	42	STO	353	32	X:T	419	54	)	485	92	RTN
156	43	RCL	222	54	)	288	10	10	354	43	RCL	420	23	LNX	486	76	LBL
157	04	04	223	95	=	289	02	2	355	11	11	421	95	=	487	19	D'
158	75	-	224	55	÷	290	55	÷	356	77	GE	422	42	STO	488	03	3
159	43	RCL	225	43	RCL	291	43	RCL	357	16	A'	423	14	14	489	05	5
160	07	07	226	10	10	292	05	05	358	76	LBL	424	76	LBL	490	69	OP
161	65	×	227	95	=	293	75	-	359	18	C'	425	15	E	491	04	04
162	53	(	228	42	STO	294	01	1	360	01	1	426	69	OP	492	43	RCL
163	43	RCL	229	11	11	295	75	-	361	44	SUM	427	00	00	493	06	06
164	04	04	230	61	GTO	296	43	RCL	362	04	04	428	43	RCL	494	69	OP
165	75	-	231	14	D	297	06	06	363	43	RCL	429	30	30	495	06	06
166	01	1	232	76	LBL	298	75	-	364	22	22	430	69	OP	496	03	3
167	54	)	233	13	C	299	43	RCL	365	69	OP	431	02	02	497	03	3
168	95	=	234	25	CLR	300	09	09	366	01	01	432	69	OP	498	69	OP
169	42	STO	235	32	X:T	301	95	=	367	43	RCL	433	05	05	499	04	04
170	08	08	236	43	RCL	302	22	INV	368	23	23	434	43	RCL	500	43	RCL
171	35	1/X	237	07	07	303	49	PRD	369	69	OP	435	14	14	501	07	07
172	65	×	238	65	×	304	10	10	370	02	02	436	99	PRT	502	69	OP
173	02	2	239	43	RCL	305	43	RCL	371	43	RCL	437	69	OP	503	06	06
174	95	=	240	06	06	306	10	10	372	26	26	438	00	00	504	98	ADV
175	75	-	241	95	=	307	22	INV	373	69	OP	439	43	RCL	505	91	R/S



Countercurrent flow in a 1-1 exchanger **Fig. 1**

tical efficiency is $F = 0.75$ to 0.80 [*1*].

When designing shell-and-tube heat exchangers in series, the lowest F value is for one shell. This value is raised as the number of shells increases, and the flow more nearly resembles countercurrent flow. The object of design is to find the minimum number of shells that will raise the F value above the chosen minimum of 0.75 to 0.80.

Determining the F factor

An article in the May 1940 issue of *The Transactions of the ASME* greatly simplified the calculations required to determine the mean temperature differences in shell-and-tube exchangers [*2*]. The equations supplied by that article have been adapted for calculator use.

The general equation, valid for any number of passes, is [*3,4*]:

$$F = \left(\frac{\sqrt{R^2+1}}{R-1}\right)\frac{\ln[(1-P_x)/(1-RP_x)]}{\ln\left[\dfrac{(2/P_x)-1-R+\sqrt{R^2+1}}{(2/P_x)-1-R-\sqrt{R^2+1}}\right]}$$

where
$$P_x = \frac{1-\left[\dfrac{RP-1}{P-1}\right]^{1/N}}{R-\left[\dfrac{RP-1}{P-1}\right]^{1/N}}$$

and
$$P = (t_2 - t_1)/(T_1 - t_1)$$
$$R = (T_1 - T_2)/(t_2 - t_1)$$

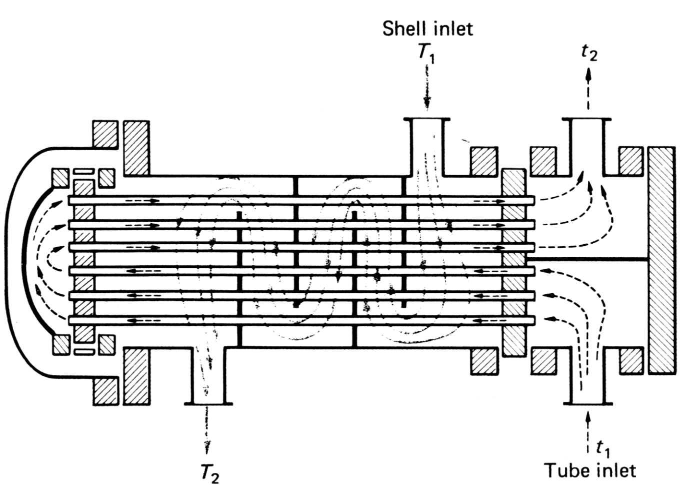
N is the total number of shell passes, i.e., the product of shell passes per shell and the number of units in series. Solving for N by repetitive trial and error with a minimum desired F, the minimum required number of shell passes can be determined.

If $R = 1$, the equation becomes indeterminate, and an alternate solution applies:

$$F = \frac{P_x\sqrt{R^2+1}/(1-P_x)}{\ln\left[\dfrac{(2/P_x)-1-R+\sqrt{R^2+1}}{(2/P_x)-1-R-\sqrt{R^2+1}}\right]}$$

and: $P_x = P/(N - NP + P)$

The equations presented are based on certain assumptions: the overall heat-transfer coefficient, U, is constant throughout the heat exchanger; the flowrate of each fluid is constant; the specific heat of each fluid is constant; there is no condensation of vapor or boiling of liquid in any part of the exchanger; heat losses are negligible; the heat-transfer surface in each pass is equal; the temperature of the shell-side fluid in any shell-side pass is uniform over any cross section.



Flow patterns in a multipass exchanger **Fig. 2**

Hewlett-Packard program
Larry Haydu

The program in Table I is written for the Hewlett-Packard HP-67/97 programmable calculators. It is simple and efficient.

The inlet and outlet temperatures of the hot and cold fluids are fed into computer memory at the start of the program. The program will select the proper number of shells in series so that the value of F is greater than or equal to 0.8. If a cutoff value for F other than 0.8 is desired, a value can be registered in the memory.

Input: T_1 [STO] 1
T_2 [STO] 2
t_1 [STO] 3
t_2 [STO] 4
F [STO] 0 (if different than 0.8)

Begin computations—Press [A]

Output is stored on the HP-67 (printed on the HP-97) and can be recalled from storage registers.

TI user instructions **Table III**

Step	Procedure	Enter	Press	Display
1.	Read in both magnetic cards, sides 1,2,3 and 4		CLR	1,2,3,4
2.	Begin computations		A	37002431
3.	Key-in hot inlet temp.	T_1	R/S	3700324137
4.	Key-in hot outlet temp.	T_2	R/S	37002431
5.	Key-in cold inlet temp.	t_1	R/S	3700324137
6.	Key-in cold outlet temp.	t_2	R/S	N
7.	Key-in number of shells (or use default value displayed)	N	R/S	Corr. LMTD
8.	Option: To calculate corrected LMTD for alternate number of shells, press B and continue with Step 7		B	N
9.	Option: Press D′ to print R and P		D′	P

Output: Number of shell passes in series — RCL A
Logarithmic mean temperature-difference (LMTD) — RCL B
Corrected mean temperature-difference (CMTD) — RCL C
Correction factor calculated (CMTD/LMTD) — RCL D

Example

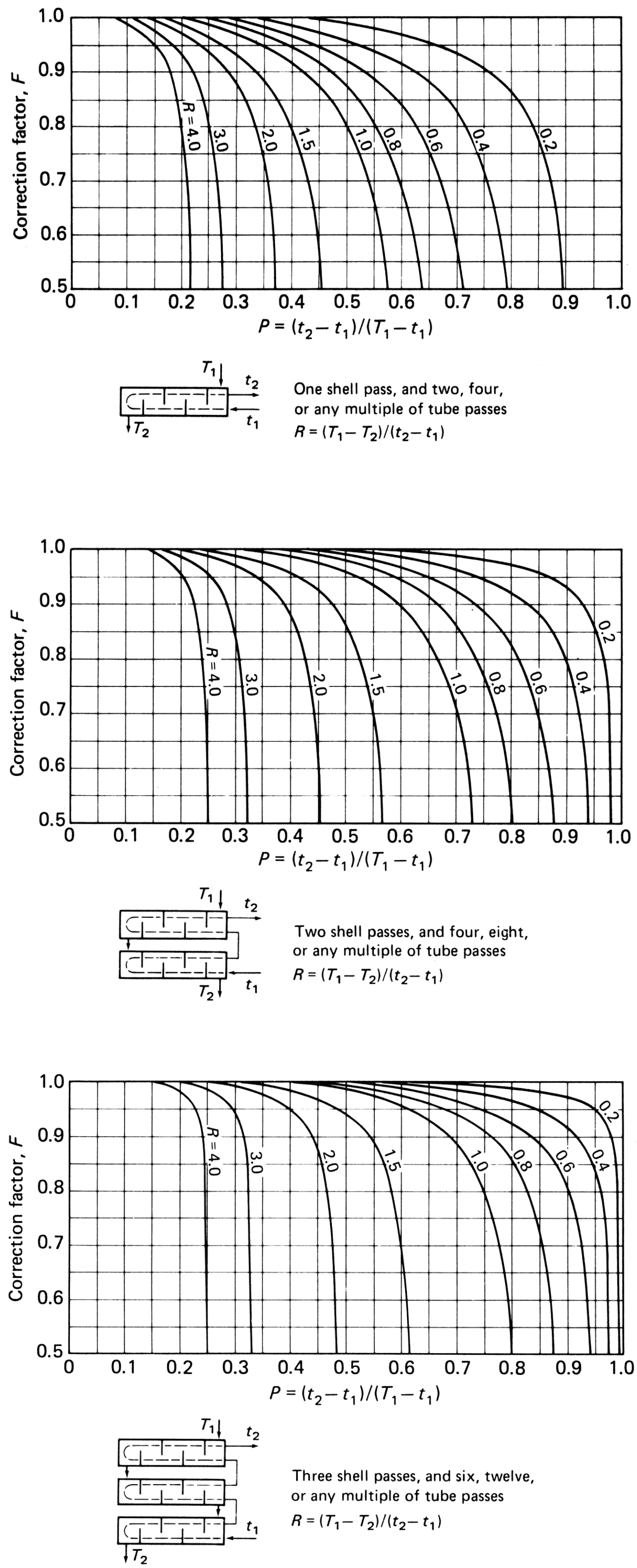
Acetone at 250°F is to be sent to storage at 100°F. The heat will be received by 100% acetic acid coming from storage at 90°F, and will raise its temperature to 150°F. Calculate the number of shell passes required, the LMTD, and the CMTD.

Answer: 3 shell passes in series required
39.09°F LMTD
34.20°F CMTD ($F = 0.87$)

TI data registers **Table IV**

0.	Hot inlet temp.--T_1	17.	1513271536
1.	Hot outlet temp.--T_2	18.	23323700
2.	Cold inlet temp.--t_1	19.	37002431
3.	Cold outlet temp.--t_2	20.	3700324137
4.	Number of shells--N	21.	1532271600
5.	P'	22.	3132400036
6.	R	23.	2317272736
7.	P	24.	1 (optional value)
8.	P''	25.	5151515151
9.	$\sqrt{R^2+1}$	26.	24311535
10.	log term	27.	1713361716
11.	F	28.	2100211315
12.	Δt_1	29.	3732350000
13.	Δt_2	30.	27303716
14.	LMTD (uncorrected)	31.	2150552730
15.	$[(PR\text{-}1)/(P\text{-}1)]^{1/N}$	32.	3716560000
16.	2730371600	33.	0.75 (optional value)

Note: The numbers in registers 16-33 are all print codes and default values that must be stored in data registers before the program is recorded on magnetic cards. The program should be recorded on magnetic cards while it is in standard partitioning.



Correction factor plot for multipass exchangers **Fig. 3**

TI user-defined keys — **Table V**

A	Starts program
B	Calculates number of shells*
C	Solves *F* factor equations*
D	Checks for minimum *F* factor*
E	Calculates corrected LMTD
A′	Calculates LMTD*
B′	Calculates LMTD if $\Delta t_1 = \Delta t_2$*
C′	Changes number of shells*
D′	Prints *R* and *P* values

*These keys all continue the program

TI example printout — **Table VI**

```
  HOT    T IN
           250.
  HOT  T OUT
           100.
COLD    T IN
            90.
COLD   T OUT
           150.
NO.  SHELLS
             1.
NO.  SHELLS INCREASED
             2.
      F FACTOR
 .6160321966
NO.  SHELLS INCREASED
             3.
      F FACTOR
 .8748644663
        LMTD
 39.08650337
      F×(LMTD)
 34.19539291
```

Texas Instruments program
W. Wayne Blackwell

The Texas Instruments program (Table II) is written for the TI-59 calculator, in conjunction with the PC-100C printer. It is completely self-prompting, calling for all necessary input data as required. This method reduces the possibility of error and confusion.

The program is largely explained by Table III (User instructions), Table IV (Data registers), and Table V (User-defined keys).

A minimum correction factor of 0.75 is used, but this may be changed at any time by keying a new value into register 33. Base −10 logs are used, as in Ref. 2.

The program is designed to start by testing one shell ($N = 1$). This minimum number of shells is known as the default number. It is possible to start with a different number by keying in any chosen value (say, $N = 3$). If this is not done, the program will start with the default number of 1. The program can be designed with a different default number (say $N = 2$) in register 24.

The program also allows the user to readily calculate the effect of a change in the number of exchanger shells on the corrected LMTD, without reentering exchanger temperatures. Just press [B], key in the number of shells desired, and then press [R/S]. The values of *R* and *P* will be printed if label [D′] is pressed.

The program may also be operated without a printer, (but, of course, in this case the self-prompting facility is lost). To do this, store exchanger temperatures (T_1, T_2, t_1 and t_2) in data registers 00 through 03, press [B], enter the estimated number of exchanger shells (or use the default value) and press [R/S]. After program execution, the results of all calculations are stored in registers 04 through 15 and can be recalled as desired. Note that the value displayed in the register at the end of a run is the corrected LMTD.

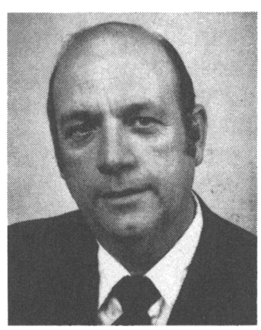
Using the previous example, start the program by pressing label [A] and answer the questions on exchanger stream temperatures as presented. The default number of shells is used as a starting point and [R/S] is pressed. The printout is shown in Table VI. The *F* value for $N = 1$ isn't a viable solution. It does not print out.

Both programs give the same result, of course.

References

1. Morton, D. S., Thermal Design of Heat Exchangers, *Ind. and Eng. Chem.*, Vol. 52, No. 6, 1960.
2. Bowman, R. A., Mueller, A. C., and Nagle, W. M., Mean Temperature Difference in Design, *Trans. ASME*, Vol. 62, 1940, pp. 283–294.
3. Taborek, J. J., Organizing Heat Exchanger Programs on Digital Computers, *Chem. Eng. Prog.*, Vol. 55, No. 10, 1959.
4. Gulley, D. L., Use Computers to Select Exchangers, *Pet. Refiner*, Vol. 39, No. 7, 1960.

The authors



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Program solves airstream energy balances

This TI-59 calculator program includes correlations for the enthalpy of air and water vapor. Thus it needs little input to solve mixing and heat-transfer energy balances and predict outlet temperatures.

Calvin R. Brunner, Malcolm Pirnie, Inc.

☐ Predicting the final temperature of two airstreams that mix, or exchange heat without mixing, involves a trial-and-error procedure because both air and water-vapor enthalpies must be considered simultaneously. This TI-59 program solves such problems quickly, using correlations for the enthalpies of air and water vapor over the range 500°F–2,500°F. Though it is most accurate over this high-temperature range, the program can be used at lower temperatures with only moderate error.

Trial-and-error

The figure illustrates the problems that this program solves:

■ Heat exchange. Given the initial temperature, air flow and water flow for two airstreams, and the final temperature for one of the streams, predict the final temperature for the other stream.

■ Mixing. Given the initial conditions as above, predict the temperature of the mixed stream.

To see how the program solves these problems, we need to look at the energy balances for each case. First, the enthalpy flow of an airstream (H_i, Btu/h) is the sum of the dry-air and water-vapor enthalpy flows:

$$H_i = [M_a h_a + M_w h_w]_i \quad (1)$$

where M is mass flowrate (1b/h), h is enthalpy (Btu/lb), a refers to air, and w refers to water.

Enthalpies h_a and h_w can be represented as functions of temperature (t, °F), based on least-squares correlations of the data shown in Table I:

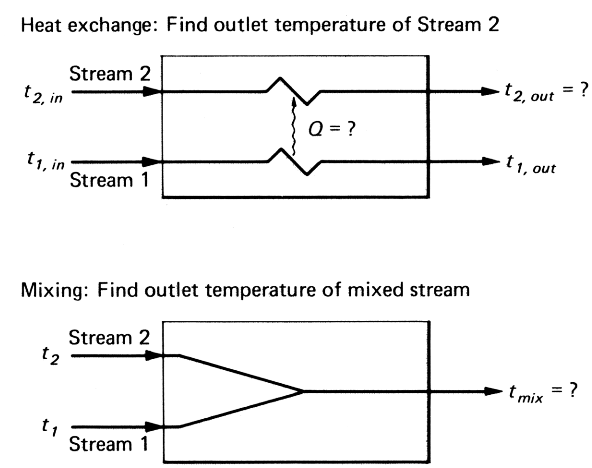
$$h_a = 0.0805\ t^{1.1506} \quad (2)$$

$$h_w = 0.56\ t + 937.8 \quad (3)$$

Substituting these equations into Eq. (1) yields the enthalpy flow for a stream of known temperature and mass flowrates.

In the case of heat exchange, both the inlet and outlet

(Text continues on p. 162)



Program handles both heat exchange and mixing **Fig. 1**

Correlations correspond closely to actual enthalpy values **Table I**

	Temperature (t), °F				
	500	1,000	1,500	2,000	2,500
Air enthalpy (h_a), Btu/lb					
Actual*	102	230	365	505	650
$h_a = 0.0805 t^{1.1506}$	103	228	363	506	654
Water-vapor enthalpy (h_w), Btu/lb					
Actual†	1,239	1,486	1,756	2,047	2,358
$h_w = 0.56 t + 937.8$	1,218	1,497	1,777	2,057	2,337

*Keenan, J. H., and Kaye, J., "Gas Tables," John Wiley & Sons, New York, 1948.
†Keenan, J. H., and Keyes, F. G., "Thermodynamic Properties of Steam," John Wiley & Sons, New York, 1936.

Originally published November 16, 1981.

Program listing for TI-59 calculator **Table II**

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
000	76	LBL	061	11	11	122	42	STO	183	01	1	244	01	1
001	24	CE	062	91	R/S	123	09	09	184	93	.	245	03	3
002	45	Y^x	063	76	LBL	124	43	RCL	185	01	1	246	02	2
003	01	1	064	18	C'	125	12	12	186	05	5	247	04	4
004	93	.	065	42	STO	126	71	SBR	187	35	1/X	248	03	3
005	01	1	066	12	12	127	24	CE	188	95	=	249	05	5
006	05	5	067	91	R/S	128	42	STO	189	42	STO	250	69	OP
007	00	0	068	76	LBL	129	13	13	190	18	18	251	04	04
008	06	6	069	19	D'	130	43	RCL	191	75	-	252	43	RCL
009	65	×	070	93	.	131	12	12	192	43	RCL	253	00	00
010	93	.	071	01	1	132	71	SBR	193	17	17	254	69	OP
011	00	0	072	32	X⇌T	133	23	LNX	194	95	=	255	06	06
012	08	8	073	43	RCL	134	42	STO	195	50	I×I	256	02	2
013	00	0	074	03	03	135	14	14	196	66	PAU	257	03	3
014	05	5	075	71	SBR	136	65	×	197	22	INV	258	07	7
015	95	=	076	24	CE	137	43	RCL	198	77	GE	259	00	0
016	92	RTN*	077	42	STO	138	11	11	199	02	02	260	03	3
017	76	LBL	078	04	04	139	85	+	200	06	06	261	02	2
018	23	LNX	079	43	RCL	140	43	RCL	201	43	RCL	262	69	OP
019	65	×	080	03	03	141	13	13	202	18	18	263	04	04
020	93	.	081	71	SBR	142	65	×	203	61	GTO	264	43	RCL
021	05	5	082	23	LNX	143	43	RCL	204	01	01	265	01	01
022	06	6	083	42	STO	144	10	10	205	53	53	266	69	OP
023	85	+	084	19	19	145	85	+	206	98	ADV	267	06	06
024	09	9	085	65	×	146	43	RCL	207	02	2	268	03	3
025	03	3	086	43	RCL	147	09	09	208	03	3	269	07	7
026	07	7	087	01	01	148	95	=	209	01	1	270	00	0
027	93	.	088	85	+	149	42	STO	210	07	7	271	00	0
028	08	8	089	43	RCL	150	16	16	211	01	1	272	02	2
029	01	1	090	04	04	151	43	RCL	212	03	3	273	04	4
030	04	4	091	65	×	152	12	12	213	69	OP	274	03	3
031	95	=	092	43	RCL	153	42	STO	214	02	02	275	01	1
032	92	RTN*	093	00	00	154	17	17	215	03	3	276	69	OP
033	76	LBL	094	95	=	155	65	×	216	07	7	277	04	04
034	11	A	095	42	STO	156	93	.	217	00	0	278	43	RCL
035	42	STO	096	05	05	157	05	5	218	00	0	279	02	02
036	00	00	097	43	RCL	158	06	6	219	03	3	280	69	OP
037	91	R/S	098	02	02	159	85	+	220	07	7	281	06	06
038	76	LBL	099	71	SBR	160	09	9	221	03	3	282	03	3
039	12	B	100	24	CE	161	03	3	222	05	5	283	07	7
040	42	STO	101	42	STO	162	08	8	223	01	1	284	03	3
041	01	01	102	06	06	163	95	=	224	03	3	285	02	2
042	91	R/S	103	43	RCL	164	65	×	225	69	OP	286	04	4
043	76	LBL	104	02	02	165	43	RCL	226	03	03	287	01	1
044	13	C	105	71	SBR	166	11	11	227	03	3	288	03	3
045	42	STO	106	23	LNX	167	94	+/-	228	01	1	289	07	7
046	02	02	107	42	STO	168	85	+	229	03	3	290	69	OP
047	91	R/S	108	07	07	169	43	RCL	230	06	6	291	04	04
048	76	LBL	109	65	×	170	16	16	231	02	2	292	43	RCL
049	14	D	110	43	RCL	171	95	=	232	01	1	293	03	03
050	42	STO	111	01	01	172	55	÷	233	01	1	294	69	OP
051	03	03	112	85	+	173	93	.	234	07	7	295	06	06
052	91	R/S	113	43	RCL	174	00	0	235	03	3	296	98	ADV
053	76	LBL	114	06	06	175	08	8	236	05	5	297	01	1
054	16	A'	115	65	×	176	00	0	237	69	OP	298	04	4
055	42	STO	116	43	RCL	177	05	5	238	04	04	299	06	6
056	10	10	117	00	00	178	55	÷	239	69	OP	300	03	3
057	91	R/S	118	75	-	179	43	RCL	240	05	05	301	02	2
058	76	LBL	119	43	RCL	180	10	10	241	98	ADV	302	03	3
059	17	B'	120	05	05	181	95	=	242	71	SBR	303	03	3
060	42	STO	121	95	=	182	45	Y^x	243	33	X^2	304	05	5

(Continued) Table II

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
305	69	OP	366	98	ADV	427	03	03	488	02	02	549	08	8
306	04	04	367	71	SBR	428	03	3	489	71	SBR	550	54	)
307	43	RCL	368	35	1/X	429	07	7	490	24	CE	551	65	×
308	09	09	369	98	ADV	430	04	4	491	42	STO	552	53	(
309	69	OP	370	98	ADV	431	03	3	492	06	06	553	43	RCL
310	06	06	371	98	ADV	432	03	3	493	43	RCL	554	01	01
311	98	ADV	372	91	R/S	433	02	2	494	02	02	555	85	+
312	71	SBR	373	76	LBL	434	00	0	495	71	SBR	556	43	RCL
313	34	ΓX	374	33	X²	435	00	0	496	23	LNX	557	11	11
314	01	1	375	03	3	436	00	0	497	42	STO	558	95	=
315	03	3	376	06	6	437	00	0	498	07	07	559	55	÷
316	02	2	377	03	3	438	69	OP	499	65	×	560	93	.
317	04	4	378	07	7	439	04	04	500	43	RCL	561	00	0
318	03	3	379	69	OP	440	69	OP	501	01	01	562	08	8
319	05	5	380	02	02	441	05	05	502	85	+	563	00	0
320	69	OP	381	03	3	442	92	RTN*	503	43	RCL	564	05	5
321	04	04	382	05	5	443	76	LBL	504	00	00	565	55	÷
322	43	RCL	383	01	1	444	35	1/X	505	65	×	566	53	(
323	10	10	384	07	7	445	05	5	506	43	RCL	567	43	RCL
324	69	OP	385	01	1	446	05	5	507	06	06	568	00	00
325	06	06	386	03	3	447	02	2	508	95	=	569	85	+
326	02	2	387	03	3	448	01	1	509	42	STO	570	43	RCL
327	03	3	388	00	0	449	02	2	510	08	08	571	10	10
328	07	7	389	00	0	450	07	7	511	43	RCL	572	95	=
329	00	0	390	00	0	451	03	3	512	12	12	573	45	Y^X
330	03	3	391	69	OP	452	02	2	513	71	SBR	574	01	1
331	02	2	392	03	03	453	04	4	514	24	CE	575	93	.
332	69	OP	393	03	3	454	03	3	515	42	STO	576	01	1
333	04	04	394	02	2	455	69	OP	516	13	13	577	05	5
334	43	RCL	395	03	3	456	02	02	517	43	RCL	578	35	1/X
335	11	11	396	01	1	457	02	2	518	12	12	579	95	=
336	69	OP	397	01	1	458	04	4	519	71	SBR	580	42	STO
337	06	06	398	07	7	459	03	3	520	23	LNX	581	15	15
338	03	3	399	00	0	460	01	1	521	42	STO	582	75	-
339	07	7	400	00	0	461	00	0	522	14	14	583	43	RCL
340	00	0	401	00	0	462	00	0	523	43	RCL	584	17	17
341	00	0	402	00	0	463	02	2	524	14	14	585	95	=
342	02	2	403	69	OP	464	07	7	525	65	×	586	50	I×I
343	04	4	404	04	04	465	69	OP	526	43	RCL	587	66	PAU
344	03	3	405	69	OP	466	03	03	527	11	11	588	22	INV
345	01	1	406	05	05	467	01	1	528	85	+	589	77	GE
346	69	OP	407	92	RTN*	468	04	4	529	43	RCL	590	05	05
347	04	04	408	76	LBL	469	06	6	530	10	10	591	99	99
348	43	RCL	409	34	ΓX	470	03	3	531	65	×	592	43	RCL
349	12	12	410	03	3	471	02	2	532	43	RCL	593	15	15
350	69	OP	411	06	6	472	03	3	533	13	13	594	42	STO
351	06	06	412	03	3	473	03	3	534	85	+	595	17	17
352	03	3	413	07	7	474	05	5	535	43	RCL	596	61	GTO
353	07	7	414	69	OP	475	05	5	536	08	08	597	05	05
354	03	3	415	02	02	476	06	6	537	75	-	598	23	23
355	02	2	416	03	3	477	69	OP	538	53	(	599	98	ADV
356	04	4	417	05	5	478	04	04	539	53	(	600	01	1
357	01	1	418	01	1	479	69	OP	540	93	.	601	05	5
358	03	3	419	07	7	480	05	05	541	05	5	602	03	3
359	07	7	420	01	1	481	92	RTN*	542	06	6	603	02	2
360	69	OP	421	03	3	482	76	LBL	543	65	×	604	69	OP
361	04	04	422	03	3	483	15	E	544	43	RCL	605	01	01
362	43	RCL	423	00	0	484	93	.	545	17	17	606	03	3
363	17	17	424	00	0	485	01	1	546	85	+	607	00	0
364	69	OP	425	00	0	486	32	X⇌T	547	09	9	608	01	1
365	06	06	426	69	OP	487	43	RCL	548	03	3	609	04	4

Table II (Continued)

Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key	Location	Code	Key
610	02	2	648	03	3	686	03	3	724	04	4	762	00	00
611	04	4	649	02	2	687	05	5	725	69	OP	763	85	+
612	03	3	650	04	4	688	69	OP	726	02	02	764	43	RCL
613	01	1	651	03	3	689	04	04	727	03	3	765	10	10
614	01	1	652	05	5	690	43	RCL	728	01	1	766	95	=
615	07	7	653	69	OP	691	10	10	729	01	1	767	69	OP
616	69	OP	654	04	04	692	69	OP	730	07	7	768	06	06
617	02	02	655	43	RCL	693	06	06	731	01	1	769	02	2
618	01	1	656	00	00	694	02	2	732	06	6	770	03	3
619	06	6	657	69	OP	695	03	3	733	00	0	771	07	7
620	00	0	658	06	06	696	07	7	734	00	0	772	00	0
621	00	0	659	02	2	697	00	0	735	03	3	773	03	3
622	01	1	660	03	3	698	03	3	736	06	6	774	02	2
623	03	3	661	07	7	699	02	2	737	69	OP	775	69	OP
624	02	2	662	00	0	700	69	OP	738	03	03	776	04	04
625	04	4	663	03	3	701	04	04	739	03	3	777	43	RCL
626	03	3	664	02	2	702	43	RCL	740	07	7	778	01	01
627	05	5	665	69	OP	703	11	11	741	03	3	779	85	+
628	69	OP	666	04	04	704	69	OP	742	05	5	780	43	RCL
629	03	03	667	43	RCL	705	06	06	743	01	1	781	11	11
630	02	2	668	01	01	706	03	3	744	07	7	782	95	=
631	01	1	669	69	OP	707	07	7	745	01	1	783	69	OP
632	02	2	670	06	06	708	69	OP	746	03	3	784	06	06
633	07	7	671	03	3	709	04	04	747	03	3	785	03	3
634	03	3	672	07	7	710	43	RCL	748	00	0	786	07	7
635	02	2	673	69	OP	711	12	12	749	69	OP	787	69	OP
636	04	4	674	04	04	712	69	OP	750	04	04	788	04	04
637	03	3	675	43	RCL	713	06	06	751	69	OP	789	43	RCL
638	69	OP	676	02	02	714	98	ADV	752	05	05	790	17	17
639	04	04	677	69	OP	715	01	1	753	01	1	791	69	OP
640	69	OP	678	06	06	716	05	5	754	03	3	792	06	06
641	05	05	679	98	ADV	717	03	3	755	02	2	793	98	ADV
642	69	OP	680	71	SBR	718	02	2	756	04	4	794	71	SBR
643	00	00	681	34	√X	719	03	3	757	03	3	795	35	1/X
644	98	ADV	682	01	1	720	00	0	758	05	5	796	98	ADV
645	71	SBR	683	03	3	721	01	1	759	69	OP	797	98	ADV
646	33	X^2	684	02	2	722	04	4	760	04	04	798	98	ADV
647	01	1	685	04	4	723	02	2	761	43	RCL	799	91	R/S

Notes: Calculator must be partitioned to 799.19 before entering the program (or reading the two program cards).

*The key shown as **RTN** must be entered as **INV SBR. RTN** appears at steps 016, 032, 407, 442 and 481.

temperatures are known for Stream 1, so $H_{1,in}$ and $H_{1,out}$ are known. From these, we can find the heat transferred to Stream 2 (Q, Btu/h):

$$Q = H_{1,in} - H_{1,out} = [M_a\,(h_{a,in} - h_{a,out}) + M_w\,(h_{w,in} - h_{w,out})]_1 \quad (4)$$

Knowing Q, we can find the outlet enthalpy flow for Stream 2:

$$H_{2,out} = Q + H_{2,in} \quad (5)$$

The program calculates Q and $H_{2,in}$ from known conditions, using Eq. (1–4), then finds $H_{2,out}$ from Eq. (5). To find the outlet temperature of Stream 2, the program uses Eq. (1–3) again and solves for t:

Stream 2 outlet:

$$t^{1.1506} = \frac{H - (0.56\,t + 937.8)\,M_w}{0.0805\,M_a} \quad (6)$$

To solve Eq. (6), the program uses a trial-and-error procedure, with 0.1°F as the tolerable error.

1. Assume a temperature value, t', and use this to calculate the right-hand side of Eq. (6).
2. Solve for t on the left-hand side of Eq. (6).
3. If $|t - t'| < 0.1$, t' is considered equal to t, and the calculation is completed.
4. If $|t - t'| \geq 0.1$, the calculated value t is substituted for t' and the program returns to Step 1.

User instructions for TI-59 program **Table III**

Step	Key	Comment
1. Partition	2 2nd OP 17	799.19
2. Enter program from Table II or from cards		
3. Enter essential data		
M_a, Stream 1	A	
M_w, Stream 1	B	
t, inlet, Stream 1	C	
M_a, Stream 2	2nd A′	
M_w, Stream 2	2nd B′	
t, inlet, Stream 2	2nd C′	
4. For mixing of two streams	E	Program runs, prints out for COMBINED FLOW
5. For heat transfer between streams		
t, outlet, Stream 1	D	
	2nd D′	Program runs, prints out for HEAT TRANSFER

Notes: While the program is running, the value $|t-t'|$ will flash in the display, decreasing each time until it is less than 0.1. At that time, the program is complete and will print out. If the printer is not used, the needed values can be recalled from the memory registers as listed in Table V.

Printouts for heat-exchange and mixing examples **Table IV**

```
HEAT TRANSFER

STREAM ONE
20000.          AIR
1500.           H²O
610.            T IN
2400.           TOUT

-11400179.83    B/HR

STREAM TWO
35000.          AIR
2850.           H²O
2450.           T IN
1483.695621     TOUT

(FLOW IN LB/HR)
```

```
COMBINED AIR FLOW

STREAM ONE
20000.          AIR
1500.           H²O
610.            T

STREAM TWO
35000.          AIR
2850.           H²O
2450.           T

COMBINED STREAM
55000.          AIR
4350.           H²O
1824.52377      T

(FLOW IN LB/HR)
```

Content of storage registers **Table V**

Register	Content
00	M_a, Stream 1, lb/h
01	M_w, Stream 1, lb/h
02	t, inlet, Stream 1, °F
03	t, outlet, Stream 1, °F
04	h_a, outlet, Stream 1, Btu/lb
05	H, outlet, Stream 1, Btu/h
06	h_a, inlet, Stream 1, Btu/lb
07	h_w, inlet, Stream 1, Btu/lb
08	Used
09	Q, Btu/h
10	M_a, Stream 2, lb/h
11	M_w, Stream 2, lb/h
12	t, inlet, Stream 2, °F
13	h_a, inlet, Stream 2, Btu/lb
14	h_w, inlet, Stream 2, Btu/lb
15	t', °F for mixed-flow case
16	H, outlet, Stream 2, Btu/h
17	t', °F for heat-transfer case
18	t, °F, final result for either case
19	h_w, outlet, Stream 1, Btu/lb

In the case where two airstreams mix, the enthalpy and mass flowrates of the mixed stream are simply the sums of the individual enthalpy and mass flowrates of the two streams:

$$H_{mix} = H_1 + H_2 \quad (7)$$

$$M_{a,mix} = M_{a,1} + M_{a,2} \quad (8)$$

$$M_{w,mix} = M_{w,1} + M_{w,2} \quad (9)$$

The program calculates these values from the given inputs, substitutes the H, M_a and M_w values for the mixed stream into Eq. (6), and solves for the temperature of the mixture by trial-and-error as above.

How to use the program

Table II lists the steps, and Table III the user instructions for the program. Note that the TI-59 calculator must be partitioned to 799.19 before entering the program (or before reading cards). If the program is used with the PC-100 printer, it prints out the relevant inputs and outputs as shown in Table IV. If the program is used without the printer, the results must be recalled from the data registers—Table V is the key to these. Register 18 holds the final result t for either mixing or heat transfer.

Example

Suppose that two airstreams are to exchange heat in a heat exchanger. The first stream is 20,000 lb/h of dry air, plus 1,500 lb/h of moisture, entering at 610°F. The second stream is 35,000 lb/h dry air, plus 2,850 lb/h moisture, entering at 2,450°F. What is the exit temperature of Stream 2 if the exit temperature of Stream 1 is assumed to be 2,400°F?

To solve this problem, partition the calculator and enter the program according to Table III. Then enter the data as shown, and press **2nd D′** to get the appropriate printout in about thirty seconds:

Airflow, Stream 1	20,000	**A**
Moisture flow, Stream 1	1,500	**B**
Inlet temperature, Stream 1	610	**C**
Airflow, Stream 2	35,000	**2nd A′**
Moisture flow, Stream 2	2,850	**2nd B′**
Inlet temperature, Stream 2	2,450	**2nd C′**
Exit temperature, Stream 1	2,400	**D**
		2nd D′

Table IV shows the resulting printout, under the heading HEAT TRANSFER. The outlet temperature of Stream 2 in this case is 1,484°F.

If the streams were to be mixed instead, the exit-temperature entry would have been unnecessary. Pressing **E** (instead of **2nd D′**) would get the program to run, and the printout would be as shown under COMBINED AIR FLOW in Table IV. In this case, the temperature of the mixed stream would be 1,824°F, as shown in Table IV.

For HP-67/97 users

The HP version closely follows the TI program. Table VI offers the HP program listing, and Table VII provides user instructions. Printouts for the examples are contained in Table VIII.

Program listing for HP version **Table VI**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	029	RCL2	36 02	057	RCL9	36 09	085	-	-45	113	1	01
002	STO2	35 02	030	GSB2	23 02	058	+	-55	086	ABS	16 31	114	.	-62
003	R↓	-31	031	RCL1	36 01	059	STOE	35 15	087	.	-62	115	1	01
004	STO1	35 01	032	×	-35	060	*LBLE	21 15	088	1	01	116	5	05
005	R↓	-31	033	ST+7	35-55 07	061	RCLE	36 15	089	X>Y?	16-34	117	0	00
006	STO0	35 00	034	RCL3	36 03	062	RCLD	36 14	090	GTO7	22 07	118	6	06
007	R/S	51	035	GSB2	23 02	063	GSB2	23 02	091	RCLI	36 46	119	yˣ	31
008	*LBLd	21 16 14	036	RCL1	36 01	064	RCL5	36 05	092	STOD	35 14	120	.	-62
009	SF1	16 21 01	037	×	-35	065	×	-35	093	GTOE	22 15	121	0	00
010	*LBLD	21 14	038	ST+8	35-55 08	066	-	-45	094	*LBL7	21 07	122	8	08
011	STO3	35 03	039	RCL7	36 07	067	.	-62	095	RCLI	36 46	123	0	00
012	STOD	35 14	040	RCL8	36 08	068	0	00	096	PRTX	-14	124	5	05
013	R↓	-31	041	-	-45	069	8	08	097	RCLA	36 11	125	×	-35
014	STO4	35 04	042	STOA	35 11	070	0	00	098	PRTX	-14	126	RTN	24
015	R↓	-31	043	RCL4	36 04	071	5	05	099	CF1	16 22 01	127	*LBL2	21 02
016	STO5	35 05	044	GSB1	23 01	072	RCL6	36 06	100	SPC	16-11	128	.	-62
017	R↓	-31	045	RCL6	36 06	073	×	-35	101	R/S	51	129	5	05
018	STO6	35 06	046	×	-35	074	÷	-24	102	*LBL4	21 04	130	6	06
019	RCL2	36 02	047	STO9	35 09	075	1	01	103	RCL1	36 01	131	×	-35
020	GSB1	23 01	048	RCL4	36 04	076	.	-62	104	ST+5	35-55 05	132	9	09
021	RCL0	36 00	049	GSB2	23 02	077	1	01	105	RCL0	36 00	133	3	03
022	×	-35	050	RCL5	36 05	078	5	05	106	ST+6	35-55 06	134	7	07
023	STO7	35 07	051	×	-35	079	0	00	107	RCL7	36 07	135	.	-62
024	RCL3	36 03	052	ST+9	35-55 09	080	6	06	108	RCL9	36 09	136	8	08
025	GSB1	23 01	053	F1?	16 23 01	081	1/X	52	109	+	-55	137	+	-55
026	RCL9	36 09	054	GTO4	22 04	082	yˣ	31	110	STOE	35 15	138	RTN	24
027	×	-35	055	*LBL3	21 03	083	STOI	35 46	111	GTOE	22 15	139	R/S	51
028	STO8	35 08	056	RCLA	36 11	084	RCLD	36 14	112	*LBL1	21 01			

User instructions for HP version **Table VII**

Air flow, lb/h, stream 1	**ENTER ↑**
Moisture flow, lb/h, stream 1	**ENTER ↑**
Inlet temperature, °F, stream 1	**Key A**
Air flow, lb/h, stream 2	**ENTER ↑**
Moisture flow, lb/h, stream 2	**ENTER ↑**
Inlet temperature, °F, stream 2	**ENTER ↑**
Exit temperature, °F, stream 1	**Key D** for heat exchange case **Key d** for mixture case

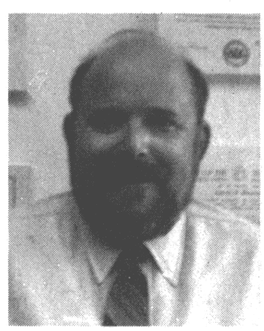
With key **D**, answer is stream 2 outlet temperature, °F.
With key **d**, answer is mixture outlet temperature, °F.

Second number in both cases is heat transfered, Btu/h.

Note: HP answers for text example differ slightly from the text TI answers. The TI program uses 1.15 for the exponent constant in Eq. (2), but the HP program uses 1.1506 as shown in the equation. Also, the TI program uses two different values for the constant 937.814 of Eq. (3), 937.814 in one case—lines 024 to 030—and 938—lines 160 to 162—in the other). The HP program uses 937.814 in both cases.

Printouts for heat-exchange and mixing examples—HP version **Table VIII**

Heat-exchange example	Mixing example
20000.00 ENT↑	20000.00 ENT↑
1500.00 ENT↑	1500.00 ENT↑
610.00 GSBA	610.00 GSBA
35000.00 ENT↑	35000.00 ENT↑
2650.00 ENT↑	2650.00 ENT↑
2450.00 ENT↑	2450.00 ENT↑
2400.00 GSBD	2400.00 GSBd
1476.95 ***	1815.37 ***
-11400179.33 ***	-11400179.23 ***



The author

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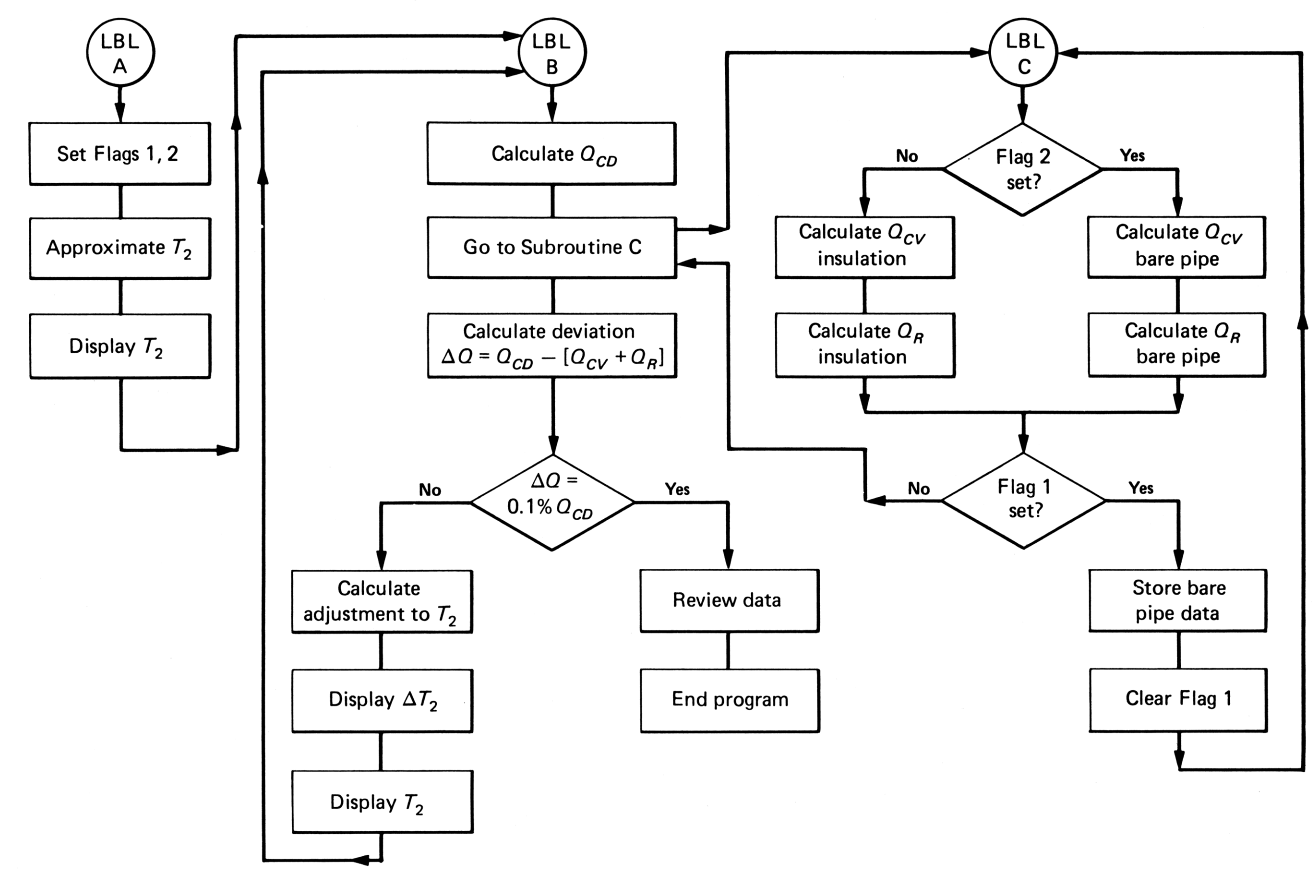
Calculating heat loss or gain by an insulated pipe

This program for the HP-97 can be used to quickly calculate the insulation surface temperature and heat loss or gain by a pipe, while all other factors are varied.

Frank S. Schroder, *3M Co.*

☐ Determining the most economical insulation system for hot or cold pipes has long been difficult to pin down without the aid of a computer because of the interdependence of the three modes of heat transfer. Charts and tables are available, but permit the evaluation of a limited range of only a few variables.

The accompanying program (figure) is developed for use with the Hewlett-Packard HP-67 or HP-97 programmable calculator, and is intended as a tool to help the engineer evaluate the parameters of: fluid temperature; ambient air temperature; thermal conductivity of the insulating material; pipe diameter; insulation thick-



Flowsheet of pipe insulation program

Originally published January 25, 1982.

Program listing

Table I

Initialize registers and flags

Step	Key	Code
001	*LBLA	21 11
002	0	00
003	STOI	35 46
004	SF1	16 21 01
005	SF2	16 21 02
006	.	-62
007	7	07
008	STOE	35 15
009	P⇄S	16-51
010	1	01
011	STO1	35 01
012	EEX	-23
013	3	03
014	STO0	35 00
015	P⇄S	16-51

First estimate of T_2

Step	Key	Code
016	RCL1	36 01
017	RCL3	36 03
018	-	-45
019	X<0?	16-45
020	SF0	16 21 00
021	F0?	16 23 00
022	CHS	-22
023	.	-62
024	5	05
025	5	05
026	Y^x	31
027	F0?	16 23 00
028	CHS	-22
029	RCL3	36 03
030	+	-55
031	STO2	35 02
032	PSE	16 51
033	*LBLB	21 12

Count iterations

Step	Key	Code
034	ISZI	16 26 46

Calculate heat conducted through insulation

Step	Key	Code
035	RCL1	36 01
036	RCL2	36 02
037	-	-45
038	2	02
039	×	-35
040	Pi	16-24
041	×	-35
042	RCL0	36 00
043	×	-35
044	RCL5	36 05
045	RCL4	36 04
046	÷	-24
047	LN	32
048	÷	-24
049	F0?	16 23 00
050	ABS	16 31
051	STO7	35 07
052	GSBC	23 13

Calculate ΔQ (error); if less than 0.1% Q_{cd}, terminate program

Step	Key	Code
053	RCL7	36 07
054	X⇄Y	-41
055	-	-45
056	STOA	35 11
057	PSE	16 51
058	RCL7	36 07
059	.	-62
060	1	01
061	%	55
062	ABS	16 31
063	RCLA	36 11
064	ABS	16 31
065	X≤Y?	16-35
066	GTOD	22 14

Calculate adjustment in T_2

Step	Key	Code
067	RCLA	36 11
068	RCL7	36 07
069	÷	-24
070	RCL4	36 04
071	RCLE	36 15
072	Y^x	31
073	RCL5	36 05
074	÷	-24
075	×	-35
076	RCL1	36 01
077	RCL2	36 02
078	-	-45
079	F0?	16 23 00
080	CHS	-22
081	RCLE	36 15
082	Y^x	31
083	F0?	16 23 00
084	CHS	-22
085	×	-35

Calculate adjustment factor F to T_2 based on convergence rate

Step	Key	Code
086	P⇄S	16-51
087	RCL0	36 00
088	X⇄Y	-41
089	STO0	35 00
090	X⇄Y	-41
091	÷	-24
092	ST+1	35-55 01

Calculate new T_2

Step	Key	Code
093	RCL1	36 01
094	RCL0	36 00
095	×	-35
096	P⇄S	16-51
097	PSE	16 51
098	ST+2	35-55 02
099	RCL2	36 02
100	PSE	16 51

Limit adjustment to T_2 to less than $(T_2 - T_3)$

Step	Key	Code
101	RCL3	36 03
102	-	-45
103	F0?	16 23 00
104	CHS	-22
105	X>0?	16-44
106	GTOB	22 12
107	1	01
108	F0?	16 23 00
109	CHS	-22
110	RCL3	36 03
111	+	-55
112	STO2	35 02
113	PSE	16 51

If overcorrection has occurred, reduce correction exponent E

Step	Key	Code
114	RCLE	36 15
115	.	-62
116	1	01
117	-	-45
118	STOE	35 15

Start recalculation

Step	Key	Code
119	GTOB	22 12

Termination of program Review data

Step	Key	Code
120	*LBLD	21 14
121	CF0	16 22 00
122	RCL2	36 02
123	PSE	16 51
124	RCL7	36 07
125	PREG	16-13
126	RTN	24
127	*LBLC	21 13

Calculate heat exchanged at surface by convection

Step	Key	Code
128	F2?	16 23 02
129	GSBc	23 16 13
130	RCL2	36 02
131	RCL3	36 03
132	-	-45
133	F0?	16 23 00
134	CHS	-22
135	RCL5	36 05
136	1	01
137	2	02
138	÷	-24
139	÷	-24
140	.	-62
141	2	02
142	5	05
143	Y^x	31
144	F0?	16 23 00
145	CHS	-22
146	.	-62
147	2	02
148	7	07
149	×	-35
150	GSBb	23 16 12
151	RCL2	36 02
152	RCL3	36 03
153	-	-45
154	×	-35
155	F0?	16 23 00
156	ABS	16 31
157	STO8	35 08

Calculate heat exchanged at surface by radiation

Step	Key	Code
158	RCL2	36 02
159	GSBa	23 16 11
160	RCL3	36 03
161	GSBa	23 16 11
162	-	-45
163	RCLC	36 13
164	×	-35
165	GSBb	23 16 12
166	.	-62
167	1	01
168	7	07
169	3	03
170	×	-35
171	F0?	16 23 00
172	ABS	16 31
173	STO9	35 09

Total heat exchanged at surface

Step	Key	Code
174	RCL8	36 08
175	+	-55
176	F1?	16 23 01
177	GTOE	22 15

Return to main program B

Step	Key	Code
178	RTN	24

Sub-routine a to calculate $\left(\frac{T_x + 460}{100}\right)^4$

Step	Key	Code
179	*LBLa	21 16 11
180	4	04
181	6	06
182	0	00
183	+	-55
184	1	01
185	0	00
186	0	00
187	÷	-24
188	4	04
189	Y^x	31
190	RTN	24

Sub-routine b ($\pi D_2/12$)

Step	Key	Code
191	*LBLb	21 16 12
192	RCL5	36 05
193	Pi	16-24
194	×	-35
195	1	01
196	2	02
197	÷	-24
198	×	-35
199	RTN	24

Sub-routine c interchanges T_1 and T_2, D_1 and D_2, e_p and e_i for purpose of calculating heat exchanged by uninsulated pipe, on first iteration

Step	Key	Code
200	*LBLc	21 16 13
201	RCL1	36 01
202	RCL2	36 02
203	STO1	35 01
204	X⇄Y	-41
205	STO2	35 02
206	RCL4	36 04
207	RCL5	36 05
208	STO4	35 04
209	X⇄Y	-41
210	STO5	35 05
211	RCLB	36 12
212	RCLC	36 13
213	STOB	35 12
214	X⇄Y	-41
215	STOC	35 13
216	RTN	24

Sub-routine E resets registers after calculating value for uninsulated pipe

Step	Key	Code
217	*LBLE	21 15
218	STO6	35 06
219	GSBc	23 16 13
220	CF1	16 22 01
221	GTOC	22 13
222	R/S	51

Typical values of thermal conductivity of insulations, Btu/(h) (ft²) (°F/ft) — Table II

	Temperature, °F					
	0	100	200	300	400	500
Fiberglass	0.010	0.011	0.020	0.023	0.031	0.043
Fiberglass - 850[1]	0.036	0.017	0.022	0.028	0.037	–
Magnesia (85%)	–	0.039	0.041	0.043	0.046	0.049
Phenolic foam[2,3]	–	–	–	0.018	–	–
Mineral wool[3]	–	–	–	0.034	–	–
Urethane foam	–	0.023	0.032	–	–	–

[1]CertainTeed
[2]Accotherm
[3]Limits not specified

Typical values of emissivity — Table III

Material	Temperature range, °F	Emissivity (*e*)
Black body	–	1.000
Aluminum—highly polished	440-1,070	0.039-0.057
—oxidized	390-1,110	0.110-0.190
Copper—polished	242	0.023
—heat-treated at 1,110 °F	390-1,110	0.570
Cast iron—heat-treated at 1,100 °F	390-1,110	0.640-0.780
Steel, oxidized at 1,100 °F	390-1,110	0.790
Nickel—polished	74	0.045
Paints—black lacquer	76	0.875
—white lacquer	100-200	0.800-0.950
—oil paints (16 colors)	212	0.920-0.960
—10%Al, 22% lacquer	212	0.520
—26%Al, 27% lacquer	212	0.300
Paper	66	0.924

ness; and emissivity of the insulation's surface. In addition, the loss or gain of a bare, uninsulated pipe is calculated for use as a reference.

The program

This program (Table I) is based on the premise that the heat conducted through the insulation, Q_{cd}, must balance the heat exchanged at the outer surface of the insulation by convection, Q_{cv}, and radiation, Q_r. For simplicity, it is assumed that the temperature of the inside of the insulation is equal to the temperature of the material inside the pipe.

The external surface temperature of the insulation is the unknown dependent variable. An estimate of this temperature is made, and the heat transferred by each of the three modes is calculated. The magnitude of the difference between Q_{cd} and $Q_{cv} + Q_r$ is determined, and is used to adjust the estimated surface temperature. This process is repeated until the figure for the heat transferred through the insulation by conduction agrees within 0.1% with the figure for the heat exchanged by convection and radiation outside the insulation.

This usually takes from three to five iterations for hot pipes, and a little more for cold ones. One of these iterations is used to calculate the heat flux of the bare, uninsulated pipe. Theoretically, requiring agreement to less than 0.1% is unwarranted, as the input data are seldom known with that degree of accuracy, and constants in the equations indicate a somewhat lower degree of precision. It is justified only in that it ensures that the calculator routine is not the limiting factor in the calculation.

User instructions for pipe insulation program — Table IV

Step	Instruction	Input Data	Keys	Output Data
1.	Clear program		f CL PRGM	
2.	Clear all storage registers		f CL REG	
3.	Enter program, either by key or by card			
4.	Store input data in primary registers:			
	Thermal conductivity, Btu/(h) (ft2) (°F) (ft)	K_m	STO 0	
	Temperature inside pipe, °F	T_1	STO 1	
	Temperature of air, °F	T_3	STO 3	
	Diameter of pipe, in.	D_1	STO 4	
	Diameter of insulation, in.	D_2	STO 5	
	Emissivity of pipe (0.79 for steel)	e_p	STO B	
	Emissivity of insulation	e_i	STO C	
5.	Run program		A	
6.	Intermediate displays—While program is running, the following information will be displayed:			
	a) Estimated surface temp. of insulation, °F			T_2
	b) ΔQ, disagreement between Q_{cd} and $Q_{cv} + Q_r$, Btu/ft			ΔQ
	c) Correction to surface temp., °F			ΔT_2
	a, b, and c will be repeated with each iteration until $\Delta Q \leqslant 0.1\% \, Q_{cd}$			
7.	At the conclusion of the program, all primary storage registers are reviewed (or printed with HP-97) to display all input and calculated data.			
8.	The calculator comes to rest with Q_{cd}, heat of conduction, in Btu/(h) (ft) in the display.			

Nomenclature

- K_m Mean thermal conductivity of insulation, Btu/(h)(ft^2)(°F)(ft) (see Table II)
- T_1 Temperature of material inside pipe, °F
- T_2 Temperature of outside surface of insulation (to be calculated by program), °F
- T_3 Temperature of ambient air, °F
- D_1 Outside diameter of pipe, in.
- D_2 Outside diameter of insulation, in.
- e Emissivity (see Table III)
- e_p Emissivity of bare pipe
- e_i Emissivity of outside surface of insulation
- Q_{cd} Heat conducted through insulation, per hour, per foot of length, Btu/(h)(ft)
- Q_{cv} Heat exchanged at surface of insulation by convection, per hour, per foot of length, Btu/(h)(ft)
- Q_r Heat exchanged at surface of insulation by radiation, per hour, per foot of length, Btu/(h)(ft)
- E Exponent used in re-estimating T_2
- F Correction factor used in re-estimating T_2
- n Number of iterations (including one to calculate values for uninsulated pipe) required to balance Q_{cd} against $Q_{cv} + Q_r$, within 0.1%.

List of storage registers **Table V**

0	K_m
1	T_1
2	T_2
3	T_3
4	D_1
5	D_2
6	$(Q_{cv} + Q_r)$ uninsulated
7	Q_{cd}
8	Q_{cv}
9	Q_r
10	ΔT
11	F
12-19	Unused
A	ΔQ
B	e_{pipe}
C	$e_{insulation}$
D	Unused
E	E (exponent)
I	n

At the conclusion of the program, all primary storage registers may be displayed or printed out, showing the input and calculated data.

This program has been used successfully to determine the effectiveness of various insulation systems under a variety of conditions, including both high and low temperatures. Results agree with published data.

If conditions are found for which the program does not readily converge, check successive intermediate displays of T_2, ΔQ and ΔT_2, to check the convergence. It is also possible to print out or display n, the number of iterations, to see if this is excessive.

The equations used in this program are:

$$Q_{cd} = \frac{2\pi K_m(T_1 - T_2)}{\ln(D_2/D_1)}$$

$$Q_{cv} = 0.27\left(\frac{T_2 - T_3}{D_2/12}\right)^{0.25}\left(\frac{\pi D_2}{12}\right)(T_2 - T_3)$$

$$Q_r = 0.173e(\pi D_2/12) \times \left[\left(\frac{T_2 + 460}{100}\right)^4 - \left(\frac{T_3 + 460}{100}\right)^4\right]$$

The definitions of terms and units are shown above. Typical values for conductivity and emissivity are listed in Tables II and III.

Steam line example

A 3-in. (3.500-in. O.D.) steel-pipe steam line carries 150 psig steam at 366°F, and is insulated with 1 in. of fiberglass insulation having a conductivity of 0.028 Btu/(h)(ft^2)(°F)(ft), and a cloth cover, painted with flat paint, having an emissivity of 0.94. The steel pipe has an emissivity of 0.79. The temperature of the surrounding air is 80°F.

Following the procedures as outlined in Table IV, it is determined that the heat loss will be 97.63 Btu/(h)(ft), and the surface temperature will be 115.2°F.

If the surface is painted with 26% aluminum paint with an emissivity of 0.30, instead of the flat paint, the heat loss will be 91.55 Btu/(h)(ft) and the surface temperature will be 130.8°F. Compare this to a heat loss of 872.4 Btu/(h)(ft) for the bare, uninsulated pipe. These calculations require four and five iterations respectively, and take less than 2 min each. Table V lists registers.

It is left for the user to determine the relative benefits of each pipe insulation system, which will depend on the prevailing economics in the local area.

For TI-58/59 users

The TI version of the program appears in Table VI. User instructions, along with data and results for the first example, are found in Table VII. Running the TI version is similar to running the HP version, but different registers are used.

In entering the data, be careful to use the diameter of the insulation (D_2), not its thickness. In the first example, the insulation is 1 in. thick, and the pipe O.D. is 3.5 in. Therefore, D_2 is 3.5 + 1 + 1 = 5.5 in. Do not use 1 in. or 4.5 in.—these certainly are incorrect!

Program listing for TI version **Table VI**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	009	43	RCL	018	59	59
001	11	A	010	05	05	019	01	1
002	00	0	011	65	×	020	42	STO
003	42	STO	012	89	π	021	11	11
004	25	25	013	55	÷	022	01	1
005	86	STF	014	01	1	023	52	EE
006	01	01	015	02	2	024	09	9
007	86	STF	016	95	=	025	42	STO
008	02	02	017	42	STO	026	10	10

(Continued) Table VI

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
027	43	RCL	091	52	EE	155	43	RCL	219	43	RCL	283	24	24
028	01	01	092	99	PRT	156	01	01	220	11	11	284	61	GTO
029	32	X:T	093	76	LBL	157	75	-	221	65	×	285	12	B
030	43	RCL	094	12	B	158	43	RCL	222	43	RCL	286	76	LBL
031	03	03	095	02	2	159	02	02	223	10	10	287	32	X:T
032	67	EQ	096	65	×	160	95	=	224	95	=	288	22	INV
033	95	=	097	53	(	161	22	INV	225	42	STO	289	86	STF
034	77	GE	098	43	RCL	162	87	IFF	226	53	53	290	00	00
035	22	INV	099	01	01	163	00	00	227	44	SUM	291	22	INV
036	76	LBL	100	75	-	164	33	X^2	228	02	02	292	52	EE
037	95	=	101	43	RCL	165	94	+/-	229	43	RCL	293	98	ADV
038	22	INV	102	02	02	166	76	LBL	230	02	02	294	43	RCL
039	87	IFF	103	54	)	167	33	X^2	231	99	PRT	295	02	02
040	00	00	104	65	×	168	45	Y^X	232	43	RCL	296	99	PRT
041	85	+	105	89	π	169	43	RCL	233	02	02	297	43	RCL
042	76	LBL	106	65	×	170	24	24	234	75	-	298	07	07
043	22	INV	107	43	RCL	171	95	=	235	43	RCL	299	99	PRT
044	86	STF	108	00	00	172	42	STO	236	03	03	300	91	R/S
045	00	00	109	55	÷	173	56	56	237	95	=	301	76	LBL
046	43	RCL	110	53	(	174	22	INV	238	42	STO	302	13	C
047	03	03	111	53	(	175	87	IFF	239	52	52	303	22	INV
048	75	-	112	43	RCL	176	00	00	240	22	INV	304	87	IFF
049	53	(	113	05	05	177	34	√X	241	87	IFF	305	02	02
050	53	(	114	55	÷	178	94	+/-	242	00	00	306	44	SUM
051	43	RCL	115	43	RCL	179	42	STO	243	35	1/X	307	71	SBR
052	03	03	116	04	04	180	56	56	244	94	+/-	308	45	Y^X
053	75	-	117	54	)	181	76	LBL	245	42	STO	309	76	LBL
054	43	RCL	118	23	LNX	182	34	√X	246	52	52	310	44	SUM
055	01	01	119	54	)	183	43	RCL	247	76	LBL	311	43	RCL
056	54	)	120	95	=	184	20	20	248	35	1/X	312	02	02
057	45	Y^X	121	42	STO	185	55	÷	249	00	0	313	75	-
058	93	.	122	07	07	186	43	RCL	250	32	X:T	314	43	RCL
059	05	5	123	22	INV	187	07	07	251	43	RCL	315	03	03
060	05	5	124	87	IFF	188	65	×	252	52	52	316	95	=
061	54	)	125	00	00	189	53	(	253	67	EQ	317	22	INV
062	95	=	126	25	CLR	190	43	RCL	254	42	STO	318	87	IFF
063	42	STO	127	50	I×I	191	04	04	255	77	GE	319	00	00
064	02	02	128	42	STO	192	45	Y^X	256	12	B	320	52	EE
065	61	GTO	129	07	07	193	43	RCL	257	76	LBL	321	94	+/-
066	23	LNX	130	76	LBL	194	24	24	258	42	STO	322	76	LBL
067	76	LBL	131	25	CLR	195	54	)	259	01	1	323	52	EE
068	85	+	132	71	SBR	196	55	÷	260	85	+	324	65	×
069	43	RCL	133	13	C	197	43	RCL	261	43	RCL	325	01	1
070	03	03	134	43	RCL	198	05	05	262	03	03	326	02	2
071	85	+	135	07	07	199	65	×	263	95	=	327	55	÷
072	53	(	136	75	-	200	43	RCL	264	42	STO	328	43	RCL
073	53	(	137	43	RCL	201	56	56	265	02	02	329	05	05
074	43	RCL	138	58	58	202	95	=	266	87	IFF	330	95	=
075	01	01	139	95	=	203	42	STO	267	00	00	331	45	Y^X
076	75	-	140	42	STO	204	55	55	268	43	RCL	332	93	.
077	43	RCL	141	20	20	205	43	RCL	269	43	RCL	333	02	2
078	03	03	142	50	I×I	206	10	10	270	03	03	334	05	5
079	54	)	143	32	X:T	207	42	STO	271	75	-	335	95	=
080	45	Y^X	144	43	RCL	208	54	54	272	01	1	336	22	INV
081	93	.	145	07	07	209	43	RCL	273	95	=	337	87	IFF
082	05	5	146	65	×	210	55	55	274	42	STO	338	00	00
083	05	5	147	93	.	211	42	STO	275	02	02	339	53	(
084	54	)	148	00	0	212	10	10	276	76	LBL	340	94	+/-
085	95	=	149	00	0	213	55	÷	277	43	RCL	341	76	LBL
086	42	STO	150	01	1	214	43	RCL	278	99	PRT	342	53	(
087	02	02	151	95	=	215	54	54	279	93	.	343	65	×
088	76	LBL	152	50	I×I	216	95	=	280	01	1	344	93	.
089	23	LNX	153	77	GE	217	44	SUM	281	22	INV	345	02	2
090	22	INV	154	32	X:T	218	11	11	282	44	SUM	346	07	7

(Continued) Table VI

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
347	65	×	373	61	GTO	399	42	STO	425	04	4	451	43	RCL
348	43	RCL	374	42	STO	400	43	43	426	06	6	452	04	04
349	59	59	375	46	46	401	22	INV	427	00	0	453	48	EXC
350	65	×	376	43	RCL	402	87	IFF	428	54	)	454	05	05
351	53	(	377	03	03	403	00	00	429	55	÷	455	42	STO
352	43	RCL	378	42	STO	404	15	E	430	01	1	456	04	04
353	02	02	379	47	47	405	50	IxI	431	00	0	457	43	RCL
354	75	-	380	71	SBR	406	76	LBL	432	00	0	458	21	21
355	43	RCL	381	61	GTO	407	15	E	433	54	)	459	48	EXC
356	03	03	382	94	+/-	408	85	+	434	45	Y×	460	22	22
357	54	)	383	85	+	409	43	RCL	435	04	4	461	42	STO
358	95	=	384	43	RCL	410	08	08	436	95	=	462	21	21
359	22	INV	385	46	46	411	95	=	437	42	STO	463	92	RTN
360	87	IFF	386	95	=	412	42	STO	438	45	45	464	76	LBL
361	00	00	387	65	×	413	58	58	439	92	RTN	465	10	E'
362	71	SBR	388	43	RCL	414	87	IFF	440	76	LBL	466	43	RCL
363	50	IxI	389	22	22	415	01	01	441	45	Y×	467	43	43
364	76	LBL	390	65	×	416	10	E'	442	22	INV	468	42	STO
365	71	SBR	391	43	RCL	417	92	RTN	443	86	STF	469	06	06
366	42	STO	392	59	59	418	76	LBL	444	02	02	470	71	SBR
367	08	08	393	65	×	419	61	GTO	445	43	RCL	471	45	Y×
368	43	RCL	394	93	.	420	53	(	446	01	01	472	22	INV
369	02	02	395	01	1	421	53	(	447	48	EXC	473	86	STF
370	42	STO	396	07	7	422	43	RCL	448	02	02	474	01	01
371	47	47	397	03	3	423	47	47	449	42	STO	475	61	GTO
372	71	SBR	398	95	=	424	85	+	450	01	01	476	13	C

User instructions and example for TI version **Table VII**

Step	Instruction	Input data	Example	Key	Output
1.	Enter program by key or card				
2.	Store input data:				
	Thermal conductivity, Btu/(h)(ft^2)(°F)(ft)	K_m	0.028	**STO 00**	
	Temperature inside pipe, °F	T_1	366	**STO 01**	
	Temperature of air, °F	T_3	80	**STO 03**	
	Diameter of pipe, in.	D_1	3.5	**STO 04**	
	Diameter of insulation, in.	D_2	5.5	**STO 05**	
	Emissivity of pipe	e_p	0.79	**STO 21**	
	Emissivity of insulation	e_i	0.94	**STO 22**	
	Calculation factor	—	0.7	**STO 24**	
3.	Run program			**A**	
4.	Intermediate printed output is surface-temperature estimates				T_2
5.	Final printout is:				
	Final surface temperature, °F	T_2			115.2
	Heat loss, Btu/(h)(ft)	Q			97.63

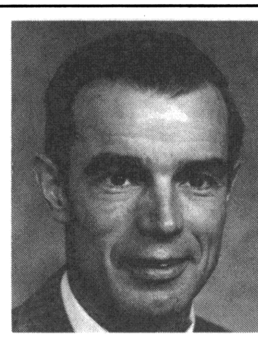
The output tape for the above example is:

```
102.4386873
111.7797835
115.0801306
115.1712315

115.1712315
97.63171797
```

References

1. Brown, G. G., et al., "Unit Operations," John Wiley & Sons, Inc., New York, 1950, pp. 427, 444, 459, 460 & 584.
2. CertainTeed Corp. Bulletin, "850° Snap-on Fiberglass Pipe Insulation," Mar. 1978.
3. Armstrong Cork Co., "Accotherm Pipe Insulation," Bulletin 15P, Nov. 1977.



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Program calculates flame temperature

Written for the HP-67 or HP-97, "FLAMTE" estimates the average temperature of a flame, and accounts for dissociation at higher temperatures.

Carl A. Vancini, *Peabody Process Systems, Inc.*

☐ Calculating the flame temperature—for a boiler, furnace or other combustor—can be a tedious trial-and-error procedure. The nature and composition of the combustion products change as the flame temperature changes. Hence, one must assume a temperature and a corresponding composition and determine whether the two match. The value finally arrived at is an average of the true temperatures that are distributed locally in a flame.

Here, a simple heat balance serves as the basis for calculating the flame temperature. The increase in enthalpy between the unburned and burned mixtures is set equal to the heat produced by the combustion.

Up to a flame temperature of about 2,500°F, the burned mixture generally includes such ordinary gases as CO_2, N_2, SO_2, H_2O and residual O_2 (from excess air). At higher temperatures, CO_2 appreciably dissociates to CO and O_2; H_2O to O_2 and OH^-; O_2 to O^{-2}; H_2 to H^+; N_2 to N^{-3}; and NO (produced by N_2 and O_2) to N^{-3} and O^{-2}. These dissociation reactions absorb an enormous amount of energy (heat), substantially lowering the flame temperature being calculated.

Heat balance

The heat balance is calculated as follows: At constant pressure, the heat, Q, required to bring the temperature of one pound of gas from temperature 0 to temperature t is:

$$Q = \int_0^t c_p \, dt \tag{1}$$

The variation of c_p with temperature can be approximated by a polynomial, having the obvious advantage of being integrated easily. Using a third-degree polynomial, we can write c_p as:

$$c_p = a + bt + ct^2 + dt^3 \tag{2}$$

where a, b, c and d are constants that depend on the nature of the gas. Eq. (1) thus becomes:

$$Q = \int_0^t (a + bt + ct^2 + dt^3) \, dt \tag{3}$$

Integrating:

$$Q = \left(a + \frac{b}{2}t + \frac{c}{3}t^2 + \frac{d}{4}t^3\right)t \tag{4}$$

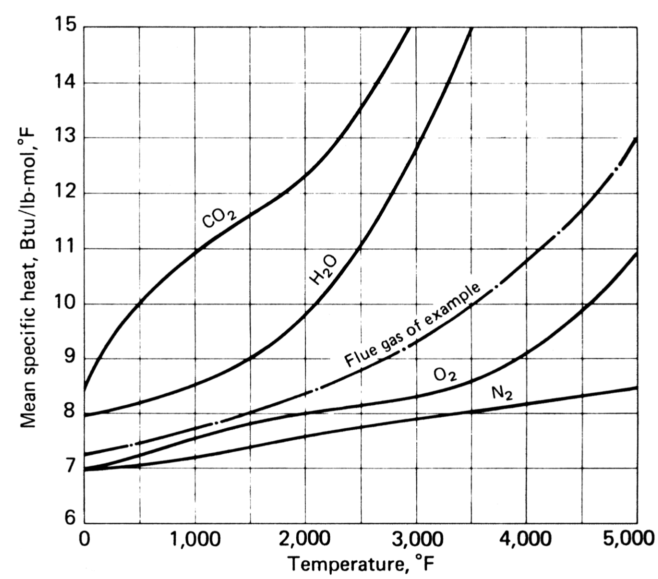
It is customary to call the parenthetic term in Eq. (4) the mean specific heat:

$$c_{pm} = a + \frac{b}{2}t + \frac{c}{3}t^2 + \frac{d}{4}t^3 \tag{5}$$

So Eq. 4 can be written as:

$$Q = c_{pm}t = at + \frac{b}{2}t^2 + \frac{c}{3}t^3 + \frac{d}{4}t^4 \tag{6}$$

By taking mean specific heats instead of the true ones, we can dispense with integration of Eq. (1). Tabulations are available of c_p and c_{pm} for many gases (not considering dissociation) [*1,2,3*].



Mean specific heats including effects of dissociation at high temperatures

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Dissociation

High-temperature dissociation of gases is a reaction that reaches equilibrium. Equilibrium depends on composition, total pressure and temperature. The degree of approach to equilibrium is also time-dependent. Tabulations of equilibrium constants for common dissociation reactions are available [4,5].

Hand calculation of the effect of dissociation on the flame temperature is extremely tedious, owing to the large number of reactions involved. For example, in the combustion of acetylene with air, one must solve a set of ten equations for ten unknown partial pressures. Here, polynomial expressions for equilibrium constants can be used [6], although with much difficulty.

Justi [7] gives values of the ratio nU/t (see nomenclature) for several dissociation reactions at various temperatures at 1 atm. Assuming a linear variation of the dissociation effects on temperature with the partial pressure of each dissociating gas, the ratio nU/t can be used to modify the mean specific heat of gases.

The figure illustrates the variation of c_{pm} with temperature, for several gases. This variation takes into account the above approach, which includes the effect of dissociation. The profiles of c_{pm} in this figure are somewhat different from those calculated by applying the modifiers of Justi. Those in the figure use more-recent thermal data and better values of calculated flame temperatures [8].

Limiting the maximum temperature to 5,000°F, a third-degree polynomial can be fitted to the curves of c_{pm} in the figure for CO_2, H_2O and O_2. For N_2, which dissociates appreciably only above 5,000°F, a second-degree polynomial is satisfactory. The coefficients are shown in Table II.

For transferring heat at constant pressure:

$$Q = \left[a(t_2 - t_1) + \frac{b}{2}(t_2^2 - t_1^2) + \frac{c}{3}(t_2^3 - t_1^3) + \frac{d}{4}(t_2^4 - t_1^4)\right]M \quad (7)$$

where Q is the heat produced by the fuel, M the amount of flue gas produced per pound of fuel, and t_1 and t_2 the initial and final temperatures, respectively.

M is also equal to the weight of fuel plus comburent (the substance that supports combustion—e.g., air or oxygen). The initial temperature, t_1, is that of the fuel and comburent mixture.

The use of Eq. (7) allows calculation of the flame temperature, t_2, by iteration via a programmable calculator. The result is not, however, to be taken at face value, but rather for comparison. This is because the actual flame temperature is always lower than the calculated one (by any method), for several reasons:

1. There is radiation and conduction to the walls of the chamber in which combustion takes place. Highly turbulent flames usually suffer an appreciable heat loss.
2. Not all of the fuel is burned. Some part may remain with the ash (as is the case for solid fuels) or escape combustion in other ways.
3. The combustion space may be of such volume or geometry that there is not enough time for all reactions of combustion and dissociation to reach equilibrium.

Nomenclature

c_p	True specific heat—Btu/lb-mol, °F; or Btu/lb, °F
c_{pm}	Mean specific heat—Btu/lb-mol, °F; or Btu/lb, °F
n	Fraction of gas dissociated
M	Flue gas produced by one pound of fuel, lb/lb
Q	Heat evolved by fuel during combustion, Btu/lb
t	Temperature, °F
t_1	Initial temperature of mixture fuel plus comburent, °F
t_2	Temperature (average) of flame, °F
U	Heat absorbed by dissociation reaction, Btu/lb-mol

In practice, the foregoing factors are usually compensated for by using an empirical coefficient. It is multiplied by the heat of combustion that is determined in the laboratory. Values of this coefficient are only estimates; this is why the flame temperature calculated with any method can only approximate actual values.

The program FLAMTE

A program called FLAMTE is written to solve Eq. (7) for t_2 (see Table I). This program is for use on the Hewlett-Packard 67 or 97. FLAMTE assumes that the flue gas contains four components: CO_2 and SO_2; O_2; H_2O; and N_2. These are determined by stoichiometry, or by an Orsat analysis for existing installations. Nitrogen is atmospheric nitrogen, and includes the argon of the air.

First, the molecular weight (wet) of the flue gas is calculated (steps 001 to 032). Then the coefficients of the mean specific heat—Eq. (5)—are calculated (coefficient a in steps 033 to 063; $b/2$, steps 064 to 091; $c/3$, steps 092 to 124; and $d/4$, steps 125 to 148). Coefficients are determined by multiplying the mole fraction by the coefficients in Table II.

The main calculation—Eq. (7)—is performed in steps 149 to 216, using the available higher combustion heat—higher heating value (HHV)—of the fuel. A simple method of iteration is used: For an initial arbitrary t_2 (the program first selects t_1 to be this), the calculator solves the right-hand side of Eq. (7) and finds the heat necessary to reach this t_2. If this heat is not equal to Q (the heat released by the fuel), t_2 is corrected accordingly and a new calculation is performed. The program iterates in this way between steps 149 and 216 until the difference between left- and right-hand sides of Eq. (7) is small enough (10°F equivalent). At this point, the value t_2 (average flame temperature) is printed (steps 217 to 222).

Running and checking the program

Table III contains the user's instructions to run FLAMTE. After entering the data and initializing by entering the preheating temperature of fuel plus comburent, **Press A** to start the program. In one or two minutes, the (average) flame temperature will be printed.

To run with another preheating temperature, just initialize with this new temperature and **Press A.** When

Written for the HP-67 or HP-97, FLAMTE quickly calculates the flame temperature **Table I**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	066	3	03	131	RCL3	36 03	196	-	-45	206	÷	-24	216	GTO1	22 01
002	STO8	35 08	067	x	-35	132	7	07	197	LSTX	16-63	207	÷	-24	217	*LBL2	21 02
003	STO5	35 05	068	STO9	35 09	133	8	08	198	STO9	35 09	208	STOI	35 46	218	RCL5	36 05
004	RCL1	36 01	069	RCL2	36 02	134	x	-35	199	.	-62	209	ABS	16 31	219	DSP0	-63 00
005	2	02	070	1	01	135	ST+9	35-55 09	200	7	07	210	1	01	220	PRTX	-14
006	8	08	071	7	07	136	RCL4	36 04	201	3	03	211	0	00	221	DSP3	-63 03
007	.	-62	072	9	09	137	6	06	202	Y^x	31	212	X>Y?	16-34	222	RTN	24
008	1	01	073	x	-35	138	7	07	203	1	01	213	GTO2	22 02	223	R/S	51
009	6	06	074	ST+9	35-55 09	139	x	-35	204	3	03	214	RCLI	36 46			
010	x	-35	075	RCL3	36 03	140	ST+9	35-55 09	205	0	00	215	ST-5	35-45 05			
011	STO0	35 00	076	EEX	-23	141	EEX	-23									
012	RCL2	36 02	077	2	02	142	1	01									
013	4	04	078	x	-35	143	4	04									
014	4	04	079	ST+9	35-55 09	144	ST÷9	35-24 09									
015	.	-62	080	RCL4	36 04	145	RCL9	36 09									
016	0	00	081	3	03	146	RCL0	36 00									
017	1	01	082	1	01	147	÷	-24									
018	x	-35	083	x	-35	148	STOD	35 14									
019	ST+0	35-55 00	084	ST-9	35-45 09	149	*LBL1	21 01									
020	RCL3	36 03	085	EEX	-23	150	RCL5	36 05									
021	3	03	086	7	07	151	RCL8	36 08									
022	2	02	087	ST÷9	35-24 09	152	-	-45									
023	x	-35	088	RCL9	36 09	153	RCLA	36 11									
024	ST+0	35-55 00	089	RCL0	36 00	154	x	-35									
025	RCL4	36 04	090	÷	-24	155	STO9	35 09									
026	1	01	091	STOB	35 12	156	RCL5	36 05									
027	8	08	092	RCL1	36 01	157	X^2	53									
028	x	-35	093	.	-62	158	RCL8	36 08									
029	ST+0	35-55 00	094	3	03	159	X^2	53									
030	EEX	-23	095	x	-35	160	-	-45									
031	2	02	096	CHS	-22	161	RCLB	36 12									
032	ST÷0	35-24 00	097	STO9	35 09	162	x	-35									
033	RCL1	36 01	098	RCL2	36 02	163	ST+9	35-55 09									
034	6	06	099	2	02	164	RCL5	36 05									
035	8	08	100	6	06	165	3	03									
036	9	09	101	.	-62	166	Y^x	31									
037	x	-35	102	3	03	167	RCL8	36 08									
038	STO9	35 09	103	x	-35	168	3	03									
039	RCL2	36 02	104	ST-9	35-45 09	169	Y^x	31									
040	8	08	105	RCL3	36 03	170	-	-45									
041	8	08	106	4	04	171	RCLC	36 13									
042	3	03	107	3	03	172	x	-35									
043	x	-35	108	.	-62	173	ST+9	35-55 09									
044	ST+9	35-55 09	109	3	03	174	RCL5	36 05									
045	RCL3	36 03	110	x	-35	175	4	04									
046	7	07	111	ST-9	35-45 09	176	Y^x	31									
047	0	00	112	RCL4	36 04	177	RCL8	36 08									
048	4	04	113	4	04	178	4	04									
049	x	-35	114	3	03	179	Y^x	31									
050	ST+9	35-55 09	115	x	-35	180	-	-45									
051	RCL4	36 04	116	ST+9	35-55 09	181	RCLD	36 14									
052	8	08	117	EEX	-23	182	x	-35									
053	1	01	118	1	01	183	ST+9	35-55 09									
054	4	04	119	0	00	184	RCL9	36 09									
055	x	-35	120	ST÷9	35-24 09	185	RCL6	36 06									
056	ST+9	35-55 09	121	RCL9	36 09	186	x	-35									
057	EEX	-23	122	RCL0	36 00	187	EEX	-23									
058	4	04	123	÷	-24	188	2	02									
059	ST÷9	35-24 09	124	STOC	35 13	189	RCL7	36 07									
060	RCL9	36 09	125	RCL2	36 02	190	-	-45									
061	RCL0	36 00	126	1	01	191	RCLE	36 15									
062	÷	-24	127	1	01	192	x	-35									
063	STOA	35 11	128	9	09	193	EEX	-23									
064	RCL1	36 01	129	x	-35	194	2	02									
065	3	03	130	STO9	35 09	195	÷	-24									

Empirical coefficients used in Eq. (5). Values account for dissociation **Table II**

Gas	*a*	*b*/2	*c*/3	*d*/4
Carbon dioxide	8.83	1.79×10^3	-2.63×10^7	1.19×10^{10}
Oxygen	7.04	1.0×10^3	-4.33×10^7	7.8×10^{11}
Water vapor	8.14	-3.1×10^4	4.3×10^7	6.7×10^{11}
Nitrogen	6.89	3.3×10^4	-3.0×10^9	–

Range of validity: 0 to 5,000°F

User's instructions for FLAMTE **Table III**

Step	Instructions	Key
Step 1	Load sides 1 and 2 of magnetic card and clear all primary registers	
Step 2	Store composition of flue gas (%, vol.):	
	N_2	**STO 1**
	CO_2 and SO_2	**STO 2**
	O_2	**STO 3**
	H_2O	**STO 4**
	(Note: Total components shall add to 100. If one component is absent, store zero)	
Step 3	Store the other data:	
	▪ Pounds of (wet) flue gas produced by 1 lb of fuel (as burned)	**STO 6**
	▪ Portion of heat (%) lost by radiation and unaccounted loss	**STO 7**
	(Note: Typical figures of loss are 1–2% for gas and oil, 2–4% for coal)	
	▪ Higher heating value of 1 lb of fuel (as burned) (Btu/lb)	**STO E**
Step 4	Initialize with the preheating temperature of comburent plus fuel (°F)	
Step 5	Run the program	**A**
	At the end of calculation time, the (average) temperature of flame will be printed	
Step 6 (optional)	Retrieve additional information:	
	Coeff. *a* of c_{pm} } Eq. (5) of flue gas (Btu/lb°F)	**RCL A**
	Coeff. *b*/2 } Eq. (5) of flue gas (Btu/lb°F)	**RCL B**
	Coeff. *c*/3 } Eq. (5) of flue gas (Btu/lb°F)	**RCL C**
	Coeff. *d*/4 } Eq. (5) of flue gas (Btu/lb°F)	**RCL D**
	Molecular weight (wet) of flue gas	**RCL 0**
	Useful higher heat value of fuel (Btu/lb)	**RCL 9**
Step 7	To run with a different preheating temperature, initialize the new temperature and go to Step 5	

Calculated and FLAMTE flame temperatures agree well for several different mixtures **Table IV**

Fuel and comburent	Higher heating value, Btu/lb	Flue gas, lb/lb fuel	Flue-gas composition, %, volume N_2	CO_2	H_2O	Flame temperature (calculated), °F	Flame temperature from FLAMTE, °F	Machine time, s
C (graphite) + air	14,140	12.52	79.10	20.90	–	3,820 [9]	3,589	64
H_2 + air	61,100	35.60	65.43	–	34.57	3,960 [9], 3,887 [11], 3,825 [8]	3,822	49
CO + air	4,368	3.47	65.43	34.57	–	3,960 [9], 3,850 [11]	3,711	84
CO + ½O_2	4,368	1.57	–	100.00	–	4,892 [8]	4,877	84
CH_4 + air	23,879	18.31	71.62	9.46	18.92	3,640 [9], 3,540 [8], 3,484 [11]	3,543*	47
CH_4 + 2O_2	23,879	5.00	–	33.33	66.67	5,150 [11], 4,959 [8]	4,982	47
C_2H_6 + air	22,320	17.16	72.60	10.96	16.44	3,710 [9], 3,540 [11]	3,595†	55
C_2H_2 + air	21,344	14.31	75.93	16.05	8.02	4,250 [9], 4,082 [8]	4,108	64
C_2H_2 + 2½ O_2	21,344	4.08	–	66.67	33.33	5,630 [11]	5,687	58
C_6H_6 (vapor) + air	18,447	14.31	75.93	16.05	8.02	3,840 [9], 3,798 [8]	3,750	63

*Observed, 3,416°F [10]; †Observed, 3,443°F [10].

Temperatures corrected for dissociation. Air or oxygen as comburent, no heat loss, initial temperatures of 60°F, stoichiometric reactions.

only the comburent is preheated to t_1 (and the fuel is at room temperature), and the specific heat of fuel and comburent are approximately the same on a pound-by-pound basis, **initialize** with t_1 multiplied by the ratio of the weight of comburent to the sum of the weights of comburent and fuel.

To verify FLAMTE, only a limited amount of flame temperature values are available from the literature (experimental values are always lower than calculated, and thus give only a first approximation). From "Gas Engineers' Handbook" [9], we have taken hand-calculated flame temperatures (corrected for dissociation) of a few compounds burned with stoichiometric air at 60°F (Table IV) and have compared them with those temperatures calculated by FLAMTE. The same has been done with flame data from Ref. [8] and Ref. [11]. Also, some observed temperatures are given for comparison. However, many old calculated values of flame temperature were based on thermal data now outdated, and are questionable.

Example

Natural gas is burned with 15% excess air. HHV = 20,614 Btu/lb; flue gas = 17.65 lb/lb of fuel; volume composition of flue gas: N_2 = 72.24%, CO_2 = 8.45%, O_2 = 2.50%, H_2O = 16.81%. Initial temperature = 70°F; unaccounted heat loss = 2%.

Following user's instructions (Table III), we introduce the following numbers:

72.24 in **Reg. 1** 17.65 in **Reg. 6**
8.45 in **Reg. 2** 2 in **Reg. 7**
2.50 in **Reg. 3** 20,614 in **Reg. E**
16.81 in **Reg. 4**

We **initialize** 70 and **Press A.** After 57 seconds of machine time, we obtain the flame temperature 3,326°F.

We can retrieve additional information:

From **Reg. A:** 0.261 = coefficient a of Eq. (5)
From **Reg. B:** $1.30 \times 10^{-5} = b/2$
From **Reg. C:** $1.33 \times 10^{-9} = c/3$
From **Reg. D:** $8.34 \times 10^{-13} = d/4$
From **Reg. O:** 27.887 = molecular weight (wet) of flue gas
From **Reg. 9:** 20,202 Btu/lb = useful HHV of fuel

Using these coefficients for c_{pm}, the variation of the mean specific heat (corrected for dissociation) versus temperature for the flue gas can be plotted (see the broken line on the figure).

For TI-58/59 users

The program listing for the TI appears in Table V. User's instructions are in Table VI—these instructions are similar as those for the HP. The example given in the HP version is repeated for the TI in Table VI.

The program will calculate and display the flame temperature. To obtain values of registers 10–13, first **Press EE.** After these values are displayed, **Press INV EE.** Otherwise, if registers 10–13 are not in the **EE** mode, the values displayed will be zero.

Program listing for TI version **Table V**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	017	43	RCL	034	44	SUM
001	11	A	018	02	02	035	00	00
002	42	STO	019	65	×	036	43	RCL
003	08	08	020	04	4	037	04	04
004	42	STO	021	04	4	038	65	×
005	05	05	022	93	.	039	01	1
006	43	RCL	023	00	0	040	08	8
007	01	01	024	01	1	041	95	=
008	65	×	025	95	=	042	44	SUM
009	02	2	026	44	SUM	043	00	00
010	08	8	027	00	00	044	01	1
011	93	.	028	43	RCL	045	52	EE
012	01	1	029	03	03	046	02	2
013	06	6	030	65	×	047	22	INV
014	95	=	031	03	3	048	49	PRD
015	42	STO	032	02	2	049	00	00
016	00	00	033	95	=	050	43	RCL

(Continued) Table V

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
051	01	01	116	19	19	181	03	3	246	43	RCL	311	54	)
052	65	×	117	43	RCL	182	95	=	247	08	08	312	65	×
053	06	6	118	03	03	183	44	SUM	248	54	)	313	43	RCL
054	08	8	119	52	EE	184	20	20	249	65	×	314	15	15
055	09	9	120	02	2	185	01	1	250	43	RCL	315	55	÷
056	95	=	121	44	SUM	186	52	EE	251	10	10	316	01	1
057	42	STO	122	19	19	187	01	1	252	95	=	317	00	0
058	09	09	123	43	RCL	188	00	0	253	42	STO	318	00	0
059	43	RCL	124	04	04	189	22	INV	254	22	22	319	95	=
060	02	02	125	65	×	190	49	PRD	255	53	(	320	42	STO
061	65	×	126	03	3	191	20	20	256	43	RCL	321	23	23
062	08	8	127	01	1	192	43	RCL	257	05	05	322	53	(
063	08	8	128	95	=	193	20	20	258	33	X^2	323	43	RCL
064	03	3	129	22	INV	194	55	÷	259	75	-	324	22	22
065	95	=	130	44	SUM	195	43	RCL	260	43	RCL	325	65	×
066	44	SUM	131	19	19	196	00	00	261	08	08	326	43	RCL
067	09	09	132	01	1	197	95	=	262	33	X^2	327	06	06
068	43	RCL	133	52	EE	198	42	STO	263	54	)	328	75	-
069	03	03	134	07	7	199	12	12	264	65	×	329	43	RCL
070	65	×	135	22	INV	200	43	RCL	265	43	RCL	330	23	23
071	07	7	136	49	PRD	201	02	02	266	11	11	331	54	)
072	00	0	137	19	19	202	65	×	267	95	=	332	55	÷
073	04	4	138	43	RCL	203	01	1	268	44	SUM	333	53	(
074	95	=	139	19	19	204	01	1	269	22	22	334	43	RCL
075	44	SUM	140	55	÷	205	09	9	270	53	(	335	23	23
076	09	09	141	43	RCL	206	95	=	271	43	RCL	336	45	Y^X
077	43	RCL	142	00	00	207	42	STO	272	05	05	337	93	.
078	04	04	143	95	=	208	21	21	273	45	Y^X	338	07	7
079	65	×	144	42	STO	209	43	RCL	274	03	3	339	03	3
080	08	8	145	11	11	210	03	03	275	75	-	340	55	÷
081	01	1	146	43	RCL	211	65	×	276	43	RCL	341	01	1
082	04	4	147	01	01	212	07	7	277	08	08	342	03	3
083	95	=	148	65	×	213	08	8	278	45	Y^X	343	00	0
084	44	SUM	149	93	.	214	95	=	279	03	3	344	54	)
085	09	09	150	03	3	215	44	SUM	280	54	)	345	95	=
086	01	1	151	94	+/-	216	21	21	281	65	×	346	42	STO
087	52	EE	152	95	=	217	43	RCL	282	43	RCL	347	16	16
088	04	4	153	42	STO	218	04	04	283	12	12	348	01	1
089	22	INV	154	20	20	219	65	×	284	95	=	349	00	0
090	49	PRD	155	43	RCL	220	06	6	285	44	SUM	350	32	X⇌T
091	09	09	156	02	02	221	07	7	286	22	22	351	43	RCL
092	43	RCL	157	65	×	222	95	=	287	53	(	352	16	16
093	09	09	158	02	2	223	44	SUM	288	43	RCL	353	50	I×I
094	55	÷	159	06	6	224	21	21	289	05	05	354	22	INV
095	43	RCL	160	93	.	225	01	1	290	45	Y^X	355	77	GE
096	00	00	161	03	3	226	52	EE	291	04	4	356	24	CE
097	95	=	162	95	=	227	01	1	292	75	-	357	43	RCL
098	42	STO	163	22	INV	228	04	4	293	43	RCL	358	16	16
099	10	10	164	44	SUM	229	22	INV	294	08	08	359	22	INV
100	43	RCL	165	20	20	230	49	PRD	295	45	Y^X	360	44	SUM
101	01	01	166	43	RCL	231	21	21	296	04	4	361	05	05
102	65	×	167	03	03	232	43	RCL	297	54	)	362	61	GTO
103	03	3	168	65	×	233	21	21	298	65	×	363	23	LNX
104	03	3	169	04	4	234	55	÷	299	43	RCL	364	76	LBL
105	95	=	170	03	3	235	43	RCL	300	13	13	365	24	CE
106	42	STO	171	93	.	236	00	00	301	95	=	366	22	INV
107	19	19	172	03	3	237	95	=	302	44	SUM	367	52	EE
108	43	RCL	173	95	=	238	42	STO	303	22	22	368	58	FIX
109	02	02	174	22	INV	239	13	13	304	53	(	369	00	00
110	65	×	175	44	SUM	240	76	LBL	305	01	1	370	43	RCL
111	01	1	176	20	20	241	23	LNX	306	00	0	371	05	05
112	07	7	177	43	RCL	242	53	(	307	00	0	372	99	PRT
113	09	9	178	04	04	243	43	RCL	308	75	-	373	58	FIX
114	95	=	179	65	×	244	05	05	309	43	RCL	374	03	03
115	44	SUM	180	04	4	245	75	-	310	07	07	375	92	RTN
												376	81	RST

User's instructions and example for TI version **Table VI**

Step	Instructions	Key
1	Enter program manually or from both sides of a magnetic card and clear registers.	CMs
2	Key in composition of flue gas (%, vol):	
	N_2	STO 01
	CO_2 and SO_2	STO 02
	O_2	STO 03
	H_2O	STO 04
3	Store the other data:	
	Pounds of (wet) flue gas produced by 1 lb of fuel (as burned)	STO 06
	Portion of heat (%) lost by radiation and unaccounted loss	STO 07
	Higher heating value of 1 lb of fuel (as burned) (Btu/lb)	STO 15
4	Key in preheating temperature of the comburent plus fuel (°F)	
5	Press **A** to run the program. At the end of calculation time the (average) temperature of flame will be printed.	A
6	Retrieve additional information (optional):	
	Coeff. *a* of c_{pm}	RCL 10
	Coeff. *b*/2 From Eq. (5), (Btu/lb °F)	EE RCL 11
	Coeff. *c*/3	RCL 12
	Coeff. *d*/4	RCL 13
	Molecular weight (wet) of flue gas	INV EE RCL 00
	Useful higher heat value of fuel (Btu/lb)	RCL 23
7	To rerun with a different preheating temperature, key in the new value and go to step 4.	A

Example:

Natural gas is burned with 15% excess air. HHV = 20,614 Btu/lb; flue gas = 17.65 lb/lb of fuel. Volume composition of flue gas: N_2 = 72.24% CO_2 = 8.45%; O_2 = 2.50%; H_2O = 16.81%. Initial temperature = 70°F; unaccounted heat loss = 2%.

Following user's instructions:

72.24	STO 01	17.65	STO 06
8.45	STO 02	2	STO 07
2.5	STO 03	20,614	STO 15
16.81	STO 04		

Initialize 70 and press **A.** After 72 s of machine time, the flame temperature is calculated to be 3,326 °F.

To retrieve additional information:

RCL 10: 0.261 = coefficient *a* of Eq. (5)
EE RCL 11: 1.30×10^{-5} = *b*/2
RCL 12: 1.33×10^{-9} = *c*/3
RCL 13: 8.34×10^{-13} = *d*/4
INV EE RCL 00: 27.887 = molecular weight (wet) of flue gas
RCL 23: 20,201.72 = useful HHV of fuel

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Calculator design of multistage evaporators

A simple mathematical model is developed by making four modest assumptions about how multistage evaporators work. The resulting Hewlett-Packard program can be used to calculate the heat-exchange area and the other significant variables.

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☐ To design multistage evaporators, we generally use iterative calculations. However, if we make the following assumptions, it is possible to achieve an analytical solution: the feed is at its boiling point; all heating surfaces are equal; sensible heats are negligible when compared with latent heats; boiling-point rise is negligible.

With these simplifications, we have developed a mathematical model and the program to solve it. The program (Table I) was run on a Hewlett-Packard 67, but it can be applied to any other HP calculator with the same type of magnetic card. The general applicability of the assumptions is discussed later on.

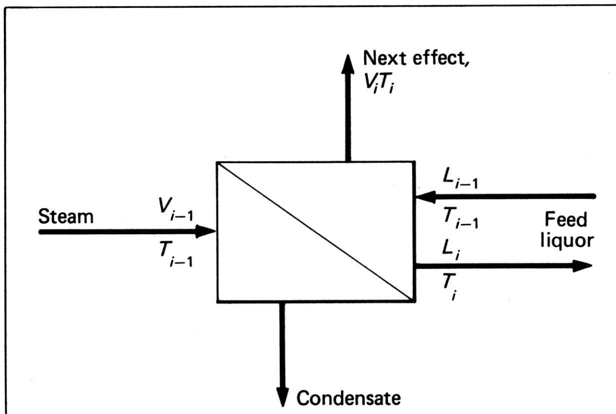
Mathematical model

Once the steady state is achieved, the mathematical model is composed of the following equations (see figure):

Material balance around Effect i:

$$L_{i-1} = L_i + V_i \tag{1}$$

$$L_{i-1}x_{i-1} = L_i x_i = L_0 x_0 = \text{constant} \tag{2}$$



Flows and temperatures for Effect *i*

Heat balance around Effect i:

$$Q_i = V_{i-1}\lambda_{i-1} \tag{3}$$

$$Q_i = U_i A(T_{i-1} - T_i) \tag{4}$$

$$Q_i = V_i\lambda_i - L_{i-1}C_{pi}(T_{i-1} - T_i) \simeq V_i\lambda_i \tag{5}$$

Hence:

$$Q_i = V_i\lambda_i = V_{i-1}\lambda_{i-1} = V_0\lambda_0 = Q = \text{constant} \tag{6}$$

and then:

$$\sum_{i=1}^{N} V_i = V_0\lambda_0 \sum_{i=1}^{N} 1/U_i = L_0 - L_N \tag{7}$$

which expresses the overall mass-balance condition. From Eq. (4) and (6):

$$Q/A = \frac{T_{i-1} - T_i}{1/U_i} = \frac{T_0 - T_N}{\sum_{i=1}^{N} 1/U_i} \tag{8}$$

Thus:

$$T_i = T_{i-1} - \left(\frac{T_0 - T_N}{\sum_{i=1}^{N} 1/U_i}\right)\left(\frac{1}{U_i}\right) \tag{9}$$

Knowing the temperatures, it is possible to evaluate the latent heat of steam, λ_i.

Applying Regnault's formula:

$$\lambda_i = 606.5 - 0.695\ T_i \tag{10}$$

where T_i is in °C, and λ_i is in kcal/kg.

Or: $$\lambda_i = 1{,}114 - 0.695\ T_i \tag{10a}$$

if T_i is in °F and λ_i is in Btu/lb.

From the independent variables—T_0, T_N, L_0, x_0, x_N and U_i—are calculated the dependent variables, which are displayed or printed by the calculator.

Originally published February 7, 1983.

Program can be used to calculate dependent variables for multistage evaporators

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
001	FIX	-11	038	GSB0	23 00	075	1/X	52	112	GSB6	23 06	149	ISZI	16 26 46	186	÷	-24
002	DSP2	-63 02	039	RCLi	36 45	076	ST+1	35-55 01	113	+	-55	150	GTOa	22 16 11	187	STOi	35 45
003	CLRG	16-53	040	P⇄S	16-51	077	P⇄S	16-51	114	RTN	24	151	*LBLb	21 16 12	188	PRTX	-14
004	P⇄S	16-51	041	ST+0	35-55 00	078	RCLI	36 46	115	R/S	51	152	RCLC	36 13	189	ISZI	16 26 46
005	CLRG	16-53	042	P⇄S	16-51	079	1	01	116	*LBLD	21 14	153	STOA	35 11	190	GTOd	22 16 14
006	CF0	16 22 00	043	GTOB	22 12	080	-	-45	117	RCL0	36 00	154	1	01	191	R/S	51
007	1	01	044	R/S	51	081	STOI	35 46	118	×	-35	155	STOI	35 46	192	*LBL5	21 05
008	STOI	35 46	045	*LBL0	21 00	082	X≠0?	16-42	119	P⇄S	16-51	156	*LBL4	21 04	193	DSZI	16 25 46
009	R/S	51	046	RCLA	36 11	083	GTO2	22 02	120	RCL0	36 00	157	RCLA	36 11	194	RCLi	36 45
010	P⇄S	16-51	047	RCL0	36 00	084	RCLi	36 45	121	GSB3	23 03	158	RCLi	36 45	195	ISZI	16 26 46
011	STO2	35 02	048	-	-45	085	GSB3	23 03	122	×	-35	159	X=0?	16-43	196	R/S	51
012	P⇄S	16-51	049	P⇄S	16-51	086	P⇄S	16-51	123	RCL0	36 00	160	GTO5	22 05	197	*LBLe	21 16 15
013	R↓	-31	050	RCL0	36 00	087	RCL1	36 01	124	ENT↑	-21	161	-	-45	198	SF0	16 21 00
014	STO0	35 00	051	÷	-24	088	×	-35	125	RCLA	36 11	162	STOA	35 11	199	R/S	51
015	R↓	-31	052	STOD	35 14	089	1/X	52	126	-	-45	163	STOi	35 45	200	*LBL6	21 06
016	STOC	35 13	053	P⇄S	16-51	090	RCLC	36 13	127	÷	-24	164	PRTX	-14	201	CLX	-51
017	R/S	51	054	0	00	091	ENT↑	-21	128	R/S	51	165	ISZI	16 26 46	202	1	01
018	X⇄Y	-41	055	STOI	35 46	092	RCLB	36 12	129	*LBLE	21 15	166	GTO4	22 04	203	1	01
019	STOA	35 11	056	RCLi	36 45	093	-	-45	130	X⇄Y	-41	167	R/S	51	204	1	01
020	X⇄Y	-41	057	*LBL1	21 01	094	×	-35	131	RCL0	36 00	168	*LBLc	21 16 13	205	4	04
021	1/X	52	058	RCLi	36 45	095	ENT↑	-21	132	GSB3	23 03	169	1	01	206	RTN	24
022	RCLC	36 13	059	ISZI	16 26 46	096	STOE	35 15	133	×	-35	170	STOI	35 46	207	R/S	51
023	×	-35	060	RCLi	36 45	097	R/S	51	134	STOD	35 14	171	RCLC	36 13			
024	P⇄S	16-51	061	X=0?	16-43	098	*LBL3	21 03	135	1	01	172	RCLB	36 12			
025	RCL2	36 02	062	GTO5	22 05	099	ENT↑	-21	136	STOI	35 46	173	-	-45			
026	×	-35	063	RCLD	36 14	100	.	-62	137	RCLC	36 13	174	RCLE	36 15			
027	P⇄S	16-51	064	×	-35	101	6	06	138	RCLD	36 14	175	÷	-24			
028	STOB	35 12	065	+	-55	102	9	09	139	R/S	51	176	R/S	51			
029	R/S	51	066	STOi	35 45	103	5	05	140	*LBLa	21 16 11	177	*LBLd	21 16 14			
030	*LBLA	21 11	067	PRTX	-14	104	CHS	-22	141	RCLD	36 14	178	RCLC	36 13			
031	1/X	52	068	GTO1	22 01	105	×	-35	142	RCLi	36 45	179	P⇄S	16-51			
032	STOi	35 45	069	*LBLC	21 13	106	6	06	143	X=0?	16-43	180	RCL2	36 02			
033	ISZI	16 26 46	070	DSZI	16 25 46	107	0	00	144	GTO5	22 05	181	×	-35			
034	R/S	51	071	*LBL2	21 02	108	6	06	145	GSB3	23 03	182	P⇄S	16-51			
035	*LBLB	21 12	072	RCLi	36 45	109	.	-62	146	÷	-24	183	RCLi	36 45			
036	DSZI	16 25 46	073	GSB3	23 03	110	5	05	147	STOi	35 45	184	X=0?	16-43			
037	X=0?	16-43	074	P⇄S	16-51	111	F0?	16 23 00	148	PRTX	-14	185	GTO5	22 05			

How to use the program

With the calculator switch in RUN position, enter the magnetic card. Then follow the instructions given below, in the same order.

1. Initialize the calculator
   Press GTO. 000
   Press R/S; in the display appears 1.00
2. Enter general data
   Key in L_0, then press ENTER
   Key in T_0, then press ENTER
   Key in x_0
   Press R/S; in the display appears L_0
   Key in T_N, then press ENTER
   Display x_N
   Press R/S; in the display appears L_N
3. Enter heat-transfer coefficients
   Key in U_1, then press A; display $1/U_1$
   Key in U_2, then press A; display $1/U_2$
   . . . .
   Key in U_N, then press A; display $1/U_N$
4. Calculate effect temperatures
   Press B; in the display appear (flashing)
   $T_1, T_2, \ldots, T_N$
   (The temperatures are still in registers 1,2,...,N, too)
5. Calculate steam consumption (1st effect)
   Press C; in the display appears . . . V_0
6. Calculate the heating surface
   Press D; in the display appears . . A
7. Calculate the heat load
   Press E; in the display appears . . . Q
8. Calculate the steam flow in each effect
   Press f a; in the display appear (flashing)
   $V_1, V_2, \ldots, V_N$
   (The steam flows are still in registers 1,2,...,N)
9. Calculate the liquid flows in each effect
   Press f b; in the display appear (flashing)
   $L_1, L_2, \ldots, L_N$
   (The liquid flows are still in registers 1,2,...,N)
10. Calculate the ratio r (steam produced/steam consumed)
    Press f c; in the display appears r
11. Calculate liquor concentrations
    Press f d; in the display appear (flashing)
    $x_1, x_2, \ldots, x_N$
    (Liquor concentrations are still in registers 1,2,...,N, too)

The program is initially devised for operating in metric units (see Nomenclature). If you wish to work in English units, then press f e; that converts the Regnault formula into these last units. This must be done at the beginning (i.e., before Key A is pressed).

Assumptions

The assumptions made for the mathematical analysis have the following limits:

The feed is at its boiling point—This is not really a limiting condition. It is only a general basis on which to compare results. If the feed is *not* at its boiling point (bp), the extra steam consumption to heat it to the boiling point can be estimated easily by hand calculations. Generally, in industrial situations, the condensed steam is used to preheat the feed in another heat exchanger, so the feed usually reaches its bp.

All the heating surfaces are equal—This is quite normal, especially in the design of industrial evaporators, due to economic considerations.

Sensible heats are negligible when compared with latent heats—This is true in the majority of the cases when the boiling-point rise (bpr) is negligible. The maximum possible error is about 20%—when the solutions are very concentrated and the bpr cannot be overlooked (see next point).

Boiling-point rise is negligible—This is the most limiting condition. It is true when the solution's molal concentration is not too high (according to Raoult's law), or when we deal with solutions of organic compounds of high molecular weights. On the other hand, when we deal with electrolytic compounds, and when the range of concentration is also very wide, the error of the estimated area can be as high as 25 to 35%.

This can be easily computed by adding the bpr of each stage (ΔT_e) and comparing this value with the thermic potential, ΔT, of the evaporator ($\Delta T = t_0 - t_N$). If $\Sigma(\Delta T_e)_i$ is 30 or 40% of ΔT, then we can expect a high level of error (35%). This error can be 40% when the number of stages is very high (7 or more).

Nevertheless, this is not a serious problem because this program is only designed to find the approximate value of the evaporation area, the most important parameter in design considerations. It is also possible to correct the area as follows:

$$A_{\text{corrected}} = A_{\text{computed}} \frac{\Delta T}{\Delta T \Sigma(\Delta T_e)_i}$$

Example

Find the value of the variables for a three-effect evaporator system.

Data:

$L_0 = 1{,}000$ kg/h; $T_0 = 100°C$; $x_0 = 0.1$;
$T_N = 60°C$; $x_N = 0.2$
$U_1 = 200$ kcal/h m^2 °C
$U_2 = 400$
$U_3 = 800$

Results:

$L_N = 500$ kg/h;
$T_1 = 77.1$ °C; $T_2 = 65.7$ °C; $T_3 = 60.0$ °C;
$V_0 = 173.6$ kg/h;
$A = 20.4\ m^2$
$Q = 93{,}243$ kcal/h
$V_1 = 168.6$ kg/h; $V_2 = 166.3$ kg/h; $V_3 = 165.1$ kg/h;
$L_1 = 831.3$ kg/h; $L_2 = 665.1$ kg/h; $L_3 = 500.0$ kg/h;
$r = 2.88$
$x_1 = 0.12$; $x_2 = 0.15$; $x_3 = 0.20$

Nomenclature

A	Heating surface, m^2 or ft^2
L_o	Feed flowrate, kg/h or lb/h
L_i	Liquor flowrate (Effect i), kg/h or lb/h
L_N	Product flowrate, kg/h or lb/h
N	Number of effects
Q	Heat load, kcal/h or Btu/h
r	Ratio between steam produced and steam consumed (dimensionless)
T_0	Steam temperature (first effect, condensation chamber), °C or °F
T_i	Liquor temperature (Effect i), °C or °F
T_N	Product temperature, °C or °F
U_i	Overall heat-transfer coefficient (Effect i), kcal/h m^2 °C or Btu/h ft^2 °F
V_0	Steam flow (first effect, condensation chamber), kg/h or lb/h
V_i	Steam flow (Effect i), kg/h or lb/h
x_0	Feed-liquor concentration (solids mass fraction), dimensionless
x_i	Liquor concentration (Effect i), dimensionless
x_N	Product concentration, dimensionless

For TI-58/59 users

The TI version of the program appears in Table II. User instructions are found in Table III, and the example is run in Table IV.

Program listing for TI version **Table II**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	023	14	14	046	43	RCL
001	10	E'	024	91	R/S	047	00	00
002	86	STF	025	42	STO	048	42	STO
003	00	00	026	15	15	049	58	58
004	01	1	027	02	2	050	43	RCL
005	01	1	028	42	STO	051	19	19
006	01	1	029	00	00	052	55	÷
007	04	4	030	91	R/S	053	43	RCL
008	42	STO	031	76	LBL	054	15	15
009	59	59	032	12	B	055	65	×
010	91	R/S	033	35	1/X	056	43	RCL
011	76	LBL	034	72	ST*	057	13	13
012	11	A	035	00	00	058	95	=
013	42	STO	036	32	X:T	059	42	STO
014	19	19	037	01	1	060	16	16
015	91	R/S	038	44	SUM	061	98	ADV
016	42	STO	039	00	00	062	99	PRT
017	01	01	040	32	X:T	063	98	ADV
018	91	R/S	041	91	R/S	064	43	RCL
019	42	STO	042	76	LBL	065	58	58
020	13	13	043	13	C	066	32	X:T
021	91	R/S	044	58	FIX	067	02	2
022	42	STO	045	02	02	068	42	STO

(Continued) Table II

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
069	00	00	133	00	00	197	01	01	261	98	ADV	325	99	PRT
070	76	LBL	134	32	X:T	198	95	=	262	42	STO	326	01	1
071	22	INV	135	43	RCL	199	65	×	263	21	21	327	44	SUM
072	73	RC*	136	58	58	200	43	RCL	264	02	2	328	00	00
073	00	00	137	75	-	201	12	12	265	42	STO	329	43	RCL
074	44	SUM	138	01	1	202	95	=	266	00	00	330	00	00
075	17	17	139	95	=	203	35	1/X	267	43	RCL	331	67	EQ
076	01	1	140	77	GE	204	65	×	268	58	58	332	45	Y^x
077	44	SUM	141	23	LNX	205	53	(	269	32	X:T	333	61	GTO
078	00	00	142	98	ADV	206	43	RCL	270	76	LBL	334	44	SUM
079	43	RCL	143	87	IFF	207	19	19	271	42	STO	335	76	LBL
080	00	00	144	00	00	208	75	-	272	43	RCL	336	45	Y^x
081	67	EQ	145	34	√X	209	43	RCL	273	21	21	337	98	ADV
082	24	CE	146	06	6	210	16	16	274	55	÷	338	53	(
083	61	GTO	147	00	0	211	54	)	275	53	(	339	43	RCL
084	22	INV	148	06	6	212	95	=	276	43	RCL	340	19	19
085	76	LBL	149	93	.	213	99	PRT	277	59	59	341	75	-
086	24	CE	150	05	5	214	98	ADV	278	75	-	342	43	RCL
087	53	(	151	42	STO	215	42	STO	279	93	.	343	16	16
088	43	RCL	152	59	59	216	20	20	280	06	6	344	54	)
089	14	14	153	76	LBL	217	65	×	281	09	9	345	55	÷
090	75	-	154	34	√X	218	43	RCL	282	05	5	346	43	RCL
091	43	RCL	155	43	RCL	219	17	17	283	65	×	347	20	20
092	01	01	156	58	58	220	65	×	284	73	RC*	348	95	=
093	54	)	157	32	X:T	221	53	(	285	00	00	349	99	PRT
094	55	÷	158	02	2	222	43	RCL	286	54	)	350	98	ADV
095	43	RCL	159	42	STO	223	59	59	287	95	=	351	02	2
096	17	17	160	00	00	224	75	-	288	99	PRT	352	42	STO
097	95	=	161	76	LBL	225	93	.	289	72	ST*	353	00	00
098	42	STO	162	33	X^2	226	06	6	290	00	00	354	76	LBL
099	18	18	163	43	RCL	227	09	9	291	01	1	355	52	EE
100	02	2	164	59	59	228	05	5	292	44	SUM	356	43	RCL
101	42	STO	165	75	-	229	65	×	293	00	00	357	19	19
102	00	00	166	93	.	230	43	RCL	294	43	RCL	358	65	×
103	76	LBL	167	06	6	231	01	01	295	00	00	359	43	RCL
104	23	LNX	168	09	9	232	54	)	296	67	EQ	360	13	13
105	73	RC*	169	05	5	233	55	÷	297	43	RCL	361	55	÷
106	00	00	170	65	×	234	53	(	298	61	GTO	362	73	RC*
107	65	×	171	73	RC*	235	43	RCL	299	42	STO	363	00	00
108	43	RCL	172	00	00	236	01	01	300	76	LBL	364	95	=
109	18	18	173	95	=	237	75	-	301	43	RCL	365	72	ST*
110	95	=	174	35	1/X	238	43	RCL	302	98	ADV	366	00	00
111	32	X:T	175	44	SUM	239	14	14	303	43	RCL	367	99	PRT
112	01	1	176	12	12	240	54	)	304	19	19	368	01	1
113	22	INV	177	01	1	241	95	=	305	42	STO	369	44	SUM
114	44	SUM	178	44	SUM	242	99	PRT	306	22	22	370	00	00
115	00	00	179	00	00	243	98	ADV	307	02	2	371	43	RCL
116	73	RC*	180	43	RCL	244	43	RCL	308	42	STO	372	00	00
117	00	00	181	00	00	245	20	20	309	00	00	373	67	EQ
118	85	+	182	67	EQ	246	65	×	310	43	RCL	374	53	(
119	32	X:T	183	35	1/X	247	53	(	311	58	58	375	61	GTO
120	95	=	184	61	GTO	248	43	RCL	312	32	X:T	376	52	EE
121	99	PRT	185	33	X^2	249	59	59	313	76	LBL	377	76	LBL
122	32	X:T	186	76	LBL	250	75	-	314	44	SUM	378	53	(
123	01	1	187	35	1/X	251	93	.	315	43	RCL	379	58	FIX
124	44	SUM	188	43	RCL	252	06	6	316	22	22	380	09	09
125	00	00	189	59	59	253	09	9	317	75	-	381	22	INV
126	32	X:T	190	75	-	254	05	5	318	73	RC*	382	86	STF
127	72	ST*	191	93	.	255	65	×	319	00	00	383	00	00
128	00	00	192	06	6	256	43	RCL	320	95	=	384	98	ADV
129	01	1	193	09	9	257	01	01	321	72	ST*	385	91	R/S
130	44	SUM	194	05	5	258	54	)	322	00	00			
131	00	00	195	65	×	259	95	=	323	42	STO			
132	43	RCL	196	43	RCL	260	99	PRT	324	22	22			

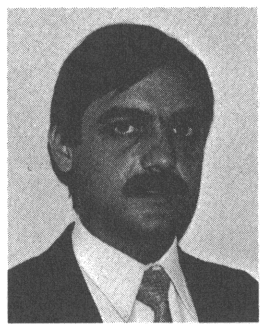
User instructions for TI version **Table III**

Step		Key	Output
1.	Clear registers	Press **CMs**	
2.	Enter data:		
	Feed flowrate, L_o	Press **A**	L_o
	Steam temperature, T_o	Press **R/S**	T_o
	Feed-liquor concentration, x_o	Press **R/S**	x_o
	Product temperature, T_N	Press **R/S**	T_N
	Product concentration, x_N	Press **R/S**	2
3.	Enter heat-transfer coefficients for each unit:		
	U_1	Press **B**	$1/U_1$
	U_2	Press **B**	$1/U_2$
Output will be:			
	Product flowrate		L_N
	Liquor temperature for each effect		T_i (i = 1 to n)
	Steam flowrate		V_o
	Heating surface		A
	Heat load		Q
	Steam flowrate for each effect		V_i (i = 1 to n)
	Liquor flowrate to each effect		L_i (i = 1 to n)
	Ratio of steam produced/consumed		r
	Liquor concentration for each effect		x_i (i = 1 to n)

Example for TI version **Table IV**

Enter	Display	Output
Data:		
1000 **A**	1000	
100 **R/S**	100	
0.1 **R/S**	0.1	
60 **R/S**	60	
0.2 **R/S**	2 (Note: 2 is displayed, not 0.2)	
200 **B**	0.005	
400 **B**	0.0025	
800 **B**	0.00125	
Run program:		
C	L_N	500.00
	T_1	77.14
	T_2	65.71
	T_3	60.00
	V_o	173.64
	A	20.40
	Q	93243.46
	V_1	168.65
	V_2	166.26
	V_3	165.09
	L_1	831.35
	L_2	665.09
	L_3	500.00
	r	2.88
	x_1	0.12
	x_2	0.15
	x_3	0.20

The authors



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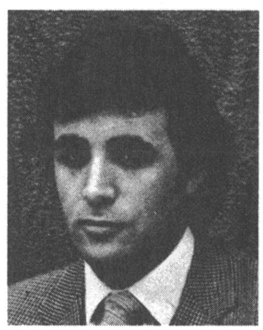

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Program for evaluation of shell-and-tube heat exchangers

With this program, it is possible to vary the design values for all the mechanical specifications and find out quickly if the designed exchanger will do the job.

Roger Crane *and* ***Robert Gregg,*** *University of South Florida*

☐ The program described here has been developed to perform the thermal and hydraulic design of standard shell-and-tube heat exchangers. Its applicability is limited to sensible heat exchange in units with normal segmented baffles *[1]*. Within these constraints, the program is quite general, accommodating a wide variety of shell and tube pass configurations.

The program (Table I) is written for the Hewlett-Packard HP-97 programmable calculator. It is designed to permit the rapid evaluation of a known heat-exchanger configuration, or to permit the rapid iteration of the design so as to obtain the optimum configuration. The user may vary the pass arrangement, tube array configurations and mechanical design parameters, and determine the effect of each on the relative thermal resistance and hydraulic performance.

Development

A suitable heat exchanger for a specific service will provide a sufficient overall heat-exchange coefficient, U, and area, A, such that the process heat load, Q, is transferred. Thus:

$$UA\,\Delta T_{eff} \geq Q \tag{1}$$

where: $\Delta T_{eff} = F_T(\text{LMTD})$

$$\text{Now } \frac{1}{U} = \frac{1}{h(D_i/D_o)} + R_{fi} + \frac{D_o \ln(D_o/D_i)}{2k_w} + R_{fo} + \frac{1}{h_o}$$

[from *2*, p. 86]

A rearrangement of these terms leads to the equation:

$$\frac{Q}{F_T(\text{LMTD})}\,\frac{1}{A} \times \left[\frac{1}{h(D_i/D_o)} + R_{fi} + \frac{D_o \ln(D_o/D_i)}{2k_w} + R_{fo} + \frac{1}{h_o}\right] \leq 1 \tag{2}$$

The five terms on the left side of the equation may be viewed as fractional thermal resistances, each one corresponding to one of the five resistances to heat transfer (Table II). In a well-sized unit, the sum of these fractional resistances approaches, but is less than, 1.

The heat-transfer correlations used in the program are taken from Kern [*2*, p. 103, 107]:

$$\frac{h_i D}{k} = 0.027\left(\frac{4m}{\pi D \mu}\right)^{0.8}\left(\frac{c_p \mu}{k}\right)^{1/3} \phi^{0.14} \tag{3}$$

$$\frac{h_o D_e}{k} = 0.36\left(\frac{M D_e}{\mu A}\right)^{0.55}\left(\frac{c_p \mu}{k}\right)^{1/3} \phi^{0.14} \tag{4}$$

Introducing Eq. 3 and 4 into Eq. 2, the individual fractional resistances may be obtained as shown in Table II. Here, the viscosity ratio, ϕ, is omitted from the tubeside and shellside convective terms. For more-viscous fluids, this term should be reintroduced prior to final sizing for greater accuracy.

Once the thermal design is optimized, the pressure drops on the shellside and tubeside are checked to ensure that they are not excessive. The equations used for calculating pressure drops are shown below [*2*, pp. 836, 839]. Both equations include frictional losses through the bundle. The tubeside term also includes typical turning losses [*2*, p. 148].

$$\Delta P_s = \frac{f_s G_s^2 D_s\left(\frac{12L}{B}\right) N_s}{5.22 \times 10^{10} D_e S_o}\,\frac{1}{\phi^{0.14}} \tag{5}$$

$$\Delta P_t = \frac{f_t G_t^2 n L}{5.22 \times 10^{10} D_i S_i}\,\frac{1}{\phi^{0.14}} + \frac{2nV_i^2}{S_i g} \tag{6}$$

In the turbulent-flow region, the friction factors may be approximated (as in Ref. 2):

$f_s = 0.0128 N_{Re}^{-0.1964}$
(straight-line portion of correlation p. 839);

$f_t = 0.0014 + 0.125 N_{Re}^{-0.32}$ (p. 53).

These correlations are incorporated in the program.

Originally published July 25, 1983.

Program

There are three parts to the program, which may be loaded onto three separate cards (Table I). Program 1 calculates the log mean temperature difference (LMTD) and the correction factor, F_T, for either a one-shell pass/two-tube pass (1–2), or a 2–4 pass arrangement. For other than a 1–2 or 2–4 pass heat exchanger, the product $F_T \times$ (LMTD) may be stored in the I register for use with Program 2.

If $F_{T,1-2} < 0.75$, or an error message is displayed, the temperature cross is too great and the 1–2 pass arrangement is not appropriate. (Temperature cross is the difference between the outlet temperature of the cold fluid and the outlet temperature of the hot fluid, when the first is higher than the second.)

Program 2 evaluates the fractional temperature drops in Table II. Each product may be printed out prior to summation. This feature is highly useful in indicating areas where design improvements can be made. Design modifications will be most beneficial in the areas where fractional resistances are relatively large.

Program 3 calculates pressure drops on the shellside and tubeside, using Eq. 5 and 6 with turbulent friction factors. The program pauses to permit incorporation of the viscosity ratio effect.

Example 1

Evaluate a 2–6 heat exchanger that uses water on the tubeside to cool 33.5° API oil. (From *[2]*, Example 8.1.)

Process conditions:

Oil inlet temp.	= 358°F
Oil outlet temp.	= 100°F
Water inlet temp.	= 90°F
Water outlet temp.	= 120°F
Oil flowrate	= 49,600 lb/h
Water flowrate	= 233,000 lb/h
Combined fouling factor	= 0.004
Allowable ΔP	= 10 psi

Heat-exchanger parameters:

Shell I.D.	= 35 in.
Baffle spacing	= 7 in.
Shell passes	= 2
No. of tubes	= 454
Length of tubes	= 12 ft
Size of tubes	= 1 in. O.D., BWG, on 1¼-in. square pitch
No. of tube passes	= 6

The combined fouling factor is referenced to the outside of the tube and therefore is calculated in the R_{fo} term. In this case, the inside fouling factor is equal to zero. The calculated value for $F_{T,2-4}$ may be used for $F_{T,2-6}$ with very little error.

Procedure

1. Load both sides of Card 1. Routine A calculates the LMTD. Routines B and C determine the LMTD correction factor, F_T, for 1–2 and 2–4 pass arrangements.

a. Store T_1, T_2, t_1, t_2 in registers b, c, d and e.

b. Push A to calculate the LMTD (71.93°F).

c. Push B to find $F_{T,1-2}$; an error is displayed, indicating conditions will not permit the use of a 1–2 unit.

d. Push CLX, then push C to find $F_{T,2-4}$ (0.92). Push R/S to store F_T (LMTD) = 66.49°F in Register I.

2. Load both sides of Card 2.

a. Store the appropriate variables in Registers R_{s0}, R_{s1}, R_{s4}–R_{s9}, R_0–R_9, R_a (see Table III). In R_8, store the value for $N_{Pr,i}$.

b. Review the stack for proper values. Ensure that R_{s3} is set to 0. Then set the primary registers to active status.

Nomenclature

A	Area for heat transfer, ft^2
B	Baffle spacing, in.
C	Tube clearance, in.
c_p	Specific heat, Btu/(lb)(°F)
D	Dia., in.
f	Friction factor
F_T	Correction factor for LMTD, depending on type of flow in the heat exchanger, dimensionless
g	Gravity acceleration, ft/s^2
G	Weight flowrate per unit area, lb/(h)(ft^2)
h	Convective heat-transfer coefficient, Btu/(h)(ft^2)(°F)
k	Thermal conductivity, Btu/(h)(ft)(°F)
L	Length of tubes for heat transfer, ft
LMTD	Log mean temperature difference for counter flow, °F
m	Weight flowrate, cold fluid, lb/h
M	Weight flowrate, hot fluid, lb/h
n	Number of tube passes
N_{Pr}	Prandtl number, dimensionless
N_{Re}	Reynolds number, dimensionless
N_s	Number of shell passes
N_t	Number of tubes per pass
P	Pressure drop, psi
P_t	Tube pitch, in.
Q	Quantity of heat transferred, Btu/h
R_A, R_B, R_C, R_D, R_E	Fractional temperature drops, dimensionless
R_f	Fouling factor, (h)(ft^2)(°F)/Btu
S	Specific gravity, dimensionless
t	Cold-fluid temperature, °F
T	Hot-fluid temperature, °F
T_{eff}	Effective temperature difference, °F
U	Overall heat-exchanger conductance, Btu/(h)(ft^2)(°F)
V	Fluid velocity, ft/s
ϕ	Ratio of viscosity measured at bulk temperature to that at wall temperature
μ	Viscosity, cP
Subscripts	
1	Inlet conditions
2	Outlet conditions
i	Inside the tube
o	Outside the tube
s	Shellside properties
e	Equivalent thermal or hydraulic diameter
w	Material properties of the tubewall
t	Tubeside properties

Vary the design specifications and find out quickly if the designed exchanger will do the job — Table I

Program 1

Step	Key	Code
001	*LBLA	21 11
002	GSB1	23 01
003	÷	-24
004	STOI	35 46
005	GSB1	23 01
006	-	-45
007	RCLI	36 46
008	LN	32
009	÷	-24
010	STO9	35 09
011	RTN	24
012	*LBL1	21 01
013	RCLB	36 12
014	RCLE	36 15
015	-	-45
016	RCLC	36 13
017	RCLD	36 14
018	-	-45
019	RTN	24
020	*LBLB	21 12
021	GSB2	23 02
022	GSB4	23 04
023	1	01
024	+	-55
025	GSB2	23 02
026	+	-55
027	GSB3	23 03
028	x	-35
029	CHS	-22
030	2	02
031	+	-55
032	STOI	35 46
033	GSB2	23 02
034	GSB4	23 04
035	CHS	-22
036	1	01
037	+	-55
038	GSB2	23 02
039	+	-55
040	GSB3	23 03
041	x	-35
042	CHS	-22
043	2	02
044	+	-55
045	RCLI	36 46
046	÷	-24
047	LN	32
048	STOI	35 46
049	GSB2	23 02
050	1	01
051	-	-45
052	RCLI	36 46
053	x	-35
054	1/X	52
055	STOI	35 46
056	GSB2	23 02
057	GSB4	23 04
058	RCLI	36 46
059	x	-35
060	STOI	35 46
061	GSB2	23 02
062	GSB3	23 03
063	x	-35
064	CHS	-22
065	1	01
066	+	-55
067	1/X	52
068	GSB3	23 03
069	CHS	-22
070	1	01
071	+	-55
072	x	-35
073	LN	32
074	RCLI	36 46
075	x	-35

Step	Key	Code
076	R/S	51
077	RCL9	36 09
078	x	-35
079	STOI	35 46
080	RTN	24
081	*LBLC	21 13
082	2	02
083	GSB3	23 03
084	÷	-24
085	1	01
086	-	-45
087	GSB2	23 02
088	-	-45
089	STOI	35 46
090	GSB5	23 05
091	GSB6	23 06
092	x	-35
093	√X	54
094	2	02
095	x	-35
096	GSB3	23 03
097	÷	-24
098	RCLI	36 46
099	+	-55
100	STO1	35 01
101	GSB2	23 02
102	GSB4	23 04
103	STO2	35 02
104	RCL1	36 01
105	+	-55
106	RCL1	36 01
107	RCL2	36 02
108	-	-45
109	÷	-24
110	LN	32
111	1/X	52
112	STOI	35 46
113	GSB6	23 06
114	STO1	35 01
115	GSB5	23 05
116	1/X	52
117	RCL1	36 01
118	x	-35
119	LN	32
120	STO1	35 01
121	GSB2	23 02
122	GSB4	23 04
123	RCL1	36 01
124	x	-35
125	2	02
126	÷	-24
127	STO1	35 01
128	GSB2	23 02
129	1	01
130	-	-45
131	1/X	52
132	RCL1	36 01
133	x	-35
134	RCLI	36 46
135	x	-35
136	R/S	51
137	RCL9	36 09
138	x	-35
139	STOI	35 46
140	RTN	24
141	*LBL6	21 06
142	GSB3	23 03
143	CHS	-22
144	1	01
145	+	-55
146	RTN	24
147	*LBL5	21 05
148	GSB2	23 02
149	GSB3	23 03
150	x	-35
151	CHS	-22

Step	Key	Code
152	1	01
153	+	-55
154	RTN	24
155	*LBL4	21 04
156	X²	53
157	1	01
158	+	-55
159	√X	54
160	RTN	24
161	*LBL3	21 03
162	RCLE	36 15
163	RCLD	36 14
164	-	-45
165	RCLB	36 12
166	RCLD	36 14
167	-	-45
168	÷	-24
169	RTN	24
170	*LBL2	21 02
171	RCLB	36 12
172	RCLC	36 13
173	-	-45
174	RCLE	36 15
175	RCLD	36 14
176	-	-45
177	÷	-24
178	RTN	24
179	R/S	51

Program 2

Step	Key	Code
001	*LBLA	21 11
002	P⇄S	16-51
003	RCL0	36 00
004	RCL4	36 04
005	÷	-24
006	P⇄S	16-51
007	.	-62
008	2	02
009	Yˣ	31
010	1	01
011	.	-62
012	1	01
013	2	02
014	x	-35
015	GSB0	23 00
016	x	-35
017	GSB1	23 01
018	RCL1	36 01
019	RCL6	36 06
020	x	-35
021	.	-62
022	8	08
023	Yˣ	31
024	x	-35
025	GSB3	23 03
026	RTN	24
027	*LBLB	21 12
028	1	01
029	.	-62
030	5	05
031	8	08
032	GSB2	23 02
033	x	-35
034	RCLA	36 11
035	x	-35
036	RCL1	36 01
037	÷	-24
038	GSB1	23 01
039	GSB3	23 03
040	RTN	24
041	*LBLC	21 13
042	.	-62
043	0	00
044	0	00
045	6	06
046	6	06

Step	Key	Code
047	8	08
048	GSB2	23 02
049	x	-35
050	P⇄S	16-51
051	RCL8	36 08
052	÷	-24
053	P⇄S	16-51
054	GSB1	23 01
055	RCL2	36 02
056	RCL1	36 01
057	÷	-24
058	LN	32
059	x	-35
060	GSB3	23 03
061	RTN	24
062	*LBLD	21 14
063	1	01
064	.	-62
065	5	05
066	8	08
067	GSB2	23 02
068	x	-35
069	P⇄S	16-51
070	RCL9	36 09
071	x	-35
072	P⇄S	16-51
073	RCL2	36 02
074	÷	-24
075	GSB1	23 01
076	GSB3	23 03
077	RTN	24
078	*LBLE	21 15
079	R/S	51
080	X=0?	16-43
081	GTO7	22 07
082	GTO6	22 06
083	*LBL7	21 07
084	GSB9	23 09
085	GTO5	22 05
086	*LBL6	21 06
087	GSB8	23 08
088	*LBL5	21 05
089	.	-62
090	4	04
091	5	05
092	Yˣ	31
093	.	-62
094	1	01
095	5	05
096	2	02
097	x	-35
098	P⇄S	16-51
099	RCL1	36 01
100	RCL5	36 05
101	÷	-24
102	.	-62
103	4	04
104	5	05
105	Yˣ	31
106	x	-35
107	P⇄S	16-51
108	RCL8	36 08
109	.	-62
110	6	06
111	7	07
112	Yˣ	31
113	x	-35
114	RCLB	36 12
115	RCLC	36 13
116	-	-45
117	x	-35
118	RCLI	36 46
119	÷	-24
120	RCL0	36 00
121	RCL3	36 03
122	x	-35

Step	Key	Code
123	RCL9	36 09
124	x	-35
125	RCL7	36 07
126	÷	-24
127	RCLE	36 15
128	÷	-24
129	.	-62
130	5	05
131	5	05
132	Yˣ	31
133	x	-35
134	GSB1	23 01
135	GSB3	23 03
136	RTN	24
137	*LBL9	21 09
138	3	03
139	.	-62
140	4	04
141	4	04
142	RCL7	36 07
143	X²	53
144	x	-35
145	Pi	16-24
146	RCL2	36 02
147	X²	53
148	x	-35
149	-	-45
150	Pi	16-24
151	÷	-24
152	RCL2	36 02
153	÷	-24
154	RTN	24
155	*LBL8	21 08
156	Pi	16-24
157	RCL2	36 02
158	X²	53
159	x	-35
160	4	04
161	÷	-24
162	CHS	-22
163	RCL7	36 07
164	X²	53
165	+	-55
166	4	04
167	x	-35
168	Pi	16-24
169	÷	-24
170	RCL2	36 02
171	÷	-24
172	RTN	24
173	*LBL2	21 02
174	P⇄S	16-51
175	RCL0	36 00
176	RCL4	36 04
177	÷	-24
178	RCL6	36 06
179	x	-35
180	P⇄S	16-51
181	RCL8	36 08
182	x	-35
183	RCLE	36 15
184	RCLD	36 14
185	-	-45
186	x	-35
187	RCLI	36 46
188	÷	-24
189	RTN	24
190	*LBL1	21 01
191	RCL4	36 04
192	÷	-24
193	RCL5	36 05
194	÷	-24
195	RCL6	36 06
196	÷	-24
197	RTN	24
198	*LBL0	21 00

Step	Key	Code
199	RCL8	36 08
200	.	-62
201	6	06
202	7	07
203	Yˣ	31
204	RCLI	36 46
205	÷	-24
206	RCLE	36 15
207	RCLD	36 14
208	-	-45
209	x	-35
210	RTN	24
211	*LBL3	21 03
212	PRTX	-14
213	P⇄S	16-51
214	RCL3	36 03
215	+	-55
216	STO3	35 03
217	P⇄S	16-51
218	RTN	24
219	R/S	51

Program 3

Step	Key	Code
001	*LBLA	21 11
002	GSB2	23 02
003	STO8	35 08
004	GSB5	23 05
005	RCL8	36 08
006	x	-35
007	P⇄S	16-51
008	RCL5	36 05
009	P⇄S	16-51
010	÷	-24
011	.	-62
012	0	00
013	3	03
014	4	04
015	4	04
016	x	-35
017	.	-62
018	1	01
019	9	09
020	6	06
021	4	04
022	CHS	-22
023	Yˣ	31
024	.	-62
025	0	00
026	1	01
027	2	02
028	8	08
029	x	-35
030	GSB5	23 05
031	X²	53
032	x	-35
033	RCL4	36 04
034	x	-35
035	RCLE	36 15
036	x	-35
037	RCL0	36 00
038	÷	-24
039	RCL3	36 03
040	x	-35
041	5	05
042	.	-62
043	2	02
044	2	02
045	EEX	-23
046	1	01
047	0	00
048	÷	-24
049	RCL8	36 08
050	1	01
051	2	02
052	÷	-24
053	÷	-24

(Continued) Table I

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
054.	P⇄S	16-51	083	*LBL1	21 01	112	4	04	141	x	-35	170	.	-62	199	P⇄S	16-51
055	RCL3	36 03	084	GSB9	23 09	113	RCL7	36 07	142	2	02	171	0	00	200	RCL2	36 02
056	P⇄S	16-51	085	GTO0	22 00	114	X²	53	143	.	-62	172	2	02	201	P⇄S	16-51
057	÷	-24	086	*LBL4	21 04	115	x	-35	144	4	04	173	8	08	202	÷	-24
058	RTN	24	087	GSB8	23 08	116	Pi	16-24	145	2	02	174	2	02	203	4	04
059	*LBL5	21 05	088	*LBL0	21 00	117	RCL2	36 02	146	÷	-24	175	x	-35	204	.	-62
060	P⇄S	16-51	089	RTN	24	118	X²	53	147	1	01	176	RCL8	36 08	205	4	04
061	RCL1	36 01	090	*LBL8	21 08	119	x	-35	148	2	02	177	X²	53	206	5	05
062	P⇄S	16-51	091	Pi	16-24	120	-	-45	149	÷	-24	178	x	-35	207	EEX	-23
063	RCL7	36 07	092	RCL2	36 02	121	Pi	16-24	150	P⇄S	16-51	179	RCL4	36 04	208	6	06
064	x	-35	093	X²	53	122	÷	-24	151	RCL4	36 04	180	x	-35	209	CHS	-22
065	RCLE	36 15	094	x	-35	123	RCL2	36 02	152	P⇄S	16-51	181	RCL5	36 05	210	x	-35
066	x	-35	095	4	04	124	÷	-24	153	÷	-24	182	x	-35	211	X²	53
067	1	01	096	÷	-24	125	RTN	24	154	.	-62	183	5	05	212	.	-62
068	4	04	097	CHS	-22	126	*LBLC	21 13	155	3	03	184	.	-62	213	0	00
069	4	04	098	RCL7	36 07	127	P⇄S	16-51	156	2	02	185	2	02	214	2	02
070	x	-35	099	X²	53	128	RCL0	36 00	157	Yˣ	31	186	2	02	215	7	07
071	RCL3	36 03	100	+	-55	129	P⇄S	16-51	158	1/X	52	187	EEX	-23	216	x	-35
072	÷	-24	101	4	04	130	1	01	159	.	-62	188	1	01	217	RCL5	36 05
073	RCL9	36 09	102	x	-35	131	8	08	160	1	01	189	0	00	218	x	-35
074	÷	-24	103	Pi	16-24	132	3	03	161	2	02	190	÷	-24	219	P⇄S	16-51
075	RCL0	36 00	104	÷	-24	133	x	-35	162	5	05	191	RCL1	36 01	220	RCL2	36 02
076	÷	-24	105	RCL2	36 02	134	RCL1	36 01	163	x	-35	192	1	01	221	P⇄S	16-51
077	RTN	24	106	÷	-24	135	X²	53	164	.	-62	193	2	02	222	÷	-24
078	*LBL2	21 02	107	RTN	24	136	÷	-24	165	0	00	194	÷	-24	223	+	-55
079	R/S	51	108	*LBL9	21 09	137	RCL6	36 06	166	0	00	195	÷	-24	224	RTN	24
080	X=0?	16-43	109	3	03	138	÷	-24	167	1	01	196	R/S	51			
081	GTO1	22 01	110	.	-62	139	STO8	35 08	168	4	04	197	÷	-24			
082	GTO4	22 04	111	4	04	140	RCL1	36 01	169	+	-55	198	RCL8	36 08			

c. Push A, B, C and then D in order, allowing time for the calculation to complete for each routine. Each fractional ΔT shown in Table II is printed out if the calculator is in the NORM position. $R_A = 0.0853$, $R_B = 0$, $R_C = 0.0034$, $R_D = 0.2955$. The sum of these products is accumulated and displayed.

d. Store the number of shell passes (2) in R_e. Store $N_{Pr,o}$ in R_8. Push E. Calculation will stop. Enter 0 for triangular tube array or 1 for square array. Push R/S. $R_E = 0.5393$ is printed out. The last number displayed is the sum of the products, $\Sigma R = 0.9235$.

This number may be used to calculate wall temperatures. The proportion of the temperature drop on the tubeside is 0.0853. The average tubeside temperature is (90 + 120)/2 = 105°F. The tubeside wall temperature will be higher than this by an amount (0.0853/0.9235) F_T(LMTD) = 6°F, i.e., T_w = 111°F. The tubeside viscosity ratio is, therefore $\phi_t = \mu_{i,105°F}/\mu_{i,111°F}$. This is approximately equal to 1.

The shellside viscosity ratio, to the fouling layer, is obtained from the average temperature of the oil—(358 + 100)/2 = 229°F—and the temperature drop across the convective layer—66.49(0.5393/0.9235) = 39°F. Hence $\phi_s = \mu_{o,(229)}/\mu_{o,(190)}$.

These values of ϕ are calculated, and R_A and R_E are each divided by the relevant ratio raised to the 0.14 power (Eq. 3,4).

The correction on the water side is negligible, but the

Calculate thermal performance of each of the five regimes to see where resistance is highest — Table II

Resistance	Numerical factor	Driving potential	Materials properties	Mechanical design	Product
Inside tube, convective	3.169	$\frac{Q}{F_T(\text{LMTD})}$	$\frac{\mu_i^{0.8}}{k_i m_i^{0.8}(N_{Pr,i})^{0.33}}$	$\frac{D_i^{0.8}}{N_t n L}$	R_A
Inside tube, fouling	$12/\pi$	$\frac{Q}{F_T(\text{LMTD})}$	$R_{f,i}$	$\frac{1}{D_i L N_t n}$	R_B
Tubewall	$1/2\pi$	$\frac{Q}{F_T(\text{LMTD})}$	$1/k_w$	$\frac{\ln(D_o/D_i)}{L N_t n}$	R_C
Outside tube, fouling	$12/\pi$	$\frac{Q}{F_T(\text{LMTD})}$	$R_{f,o}$	$\frac{1}{D_o L N_t n}$	R_D
Outside tube, convective	0.367	$\frac{Q}{F_T(\text{LMTD})}$	$\frac{\mu_o^{0.55}}{k_o m_o^{0.55}(N_{Pr,o})^{0.33}}$	$\frac{D_e^{0.45}(BD_sC)^{0.55}}{D_o L N_t n(P_t N_s)^{0.55}}$	R_E
				ΣProducts	ΣR

Contents of registers for Example 1 **Table III**

Secondary storage register	Variable	Numerical value	Primary storage register	Variable	Numerical value
R_{s0}	m_i	233,000 lb/h	R_0	B	7 in.
R_{s1}	m_o	49,600 lb/h	R_1	D_i	0.76 in.
R_{s2}	S_i	1.0	R_2	D_o	1.0 in.
R_{s3}	S_o	0.82	R_3	D_s	35 in.
R_{s4}	μ_i	0.73 cP	R_4	L	12 ft
R_{s5}	μ_o	1.12 cP	R_5	n	6
R_{s6}	k_i	0.37 Btu/(h)(ft)(°F)	R_6	N_t	$\frac{454}{6} = 75.67$
R_{s7}	k_o	0.076 Btu/(h)(ft)(°F)			
R_{s8}	k_w	25 Btu/(h)(ft)(°F)	R_7	P_t	1.25 in. (square array)
R_{s9}	$R_{f,o}$	0.004			
			R_8	$N_{Pr,i}(N_{Pr,o})$	4.78 (18.22)
			R_9	C	0.25 in.

Register	Variable	Value
R_a	$R_{f,i}$	0
R_b	T_1	358°F
R_c	T_2	100°F
R_d	t_1	90°F
R_e	t_2, (N_s)	120°F, (2)
I	F_t(LMTD)	Calculated by program

viscosity of 33.5° API oil is found to be 1.95 cP at 190°F. Therefore, $R_E = 0.5393/(1.12/1.95)^{0.14} = 0.5393/0.9253 = 0.5828$. The revised sum of products is 0.967, which is still less than 1, and hence the thermal design is fine.

If Σ products ≤ 1.0, continue to Step 3. Otherwise, the heat-exchanger design must be modified to obtain sufficient thermal performance.

3. Load both sides of Program 3.

a. Store S_i in R_{s2}, store S_o in R_{s3}. Return to primary registers.

b. Push A. When calculation stops, enter 0 for triangular array or 1 for square array. Push R/S to continue. $\Delta P_s = 6.21$ psi is displayed. $\Delta P_s < 10.0$ psi, which is acceptable. Divide by $\phi_s^{0.14}$. $\Delta P_s = 6.71$, still acceptable.

c. Push C. When the program stops, enter $\phi_t^{0.14}$ and push R/S. $\Delta P_t < 10.0$ psi, which is satisfactory.

Example 2

As a further example of the design procedure, again use the data of Example 1, but design for a fouling factor of $R_f = 0.003$ instead of 0.004. Any-size unit may be tried for the initial estimate. For convenience, start with the same unit used in Example 1.

1. The F_T and LMTD values remain unchanged; $F_{T,2\text{-}4} = 0.92$, LMTD = 71.93°F.

2. The uncorrected fractional temperature drops are: $R_A = 0.0853$, $R_B = 0$, $R_c = 0.0034$, $R_D = 0.2216$, $R_E = 0.5393$, $\Sigma R = 0.8496$.

a. The unit is oversized by about 15%. Size may be decreased by using a smaller-diameter shell or a shorter tube bundle. If the pressure drop permits, the smaller shell size will generally result in the lower-cost unit.

b. For the next iteration, try a 31-in. shell. Tube-count tables [2] suggest that up to 368 tubes may be included in this size of shell.

Adjust the registers so that $R_3 = 31$ in. and $R_6 = 368/6$ (61.33). Repeating the calculations on Card 2, we find the following unadjusted fractional temperature drops: $R_A = 0.0890$, $R_B = 0$, $R_C = 0.0042$, $R_D = 0.2734$, $R_E = 0.6224$ and $\Sigma R = 0.9890$. The shellside wall temperature may be calculated at 187°F, for a wall viscosity of 2 cP. The corrected $\Sigma R = 1.038$.

The unit is now thermally too small. The major resistance is still on the shellside. Decreasing the baffle spacing would improve heat transfer by increasing turbulence. The minimum baffle spacing permitted by TEMA is 20% of the small diameter, or 6.2 in.

c. Set $R_0 = 6.2$, then rerun. Now $R_A = 0.0890$, $R_B = 0$, $R_C = 0.0042$, $R_D = 0.2734$, $R_E = 0.5822$. After applying the correction factor on viscosity, $R_E = 0.6314$ and $\Sigma R = 0.9980$. The unit is of adequate size.

3. Check the pressure drop on the new unit. $\Delta P_s = 10.39$, $\Delta P_t = 9.55$ psi. The shellside is slightly high but probably within the acceptable range.

For TI-58/59 users

The TI version closely follows the HP program. There are 3 TI programs (see listings in Tables IV, V and VI, respectively); and user instruction are offered in Table VII. A printout of the first example can be seen in Table VIII.

Listing for TI version—program A **Table IV**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	033	95	=	066	75	-
001	11	A	034	42	STO	067	43	RCL
002	43	RCL	035	29	29	068	23	23
003	21	21	036	99	PRT	069	54	)
004	75	-	037	53	(	070	95	=
005	43	RCL	038	43	RCL	071	42	STO
006	24	24	039	21	21	072	28	28
007	95	=	040	75	-	073	43	RCL
008	42	STO	041	43	RCL	074	29	29
009	25	25	042	22	22	075	91	R/S
010	43	RCL	043	54	)	076	76	LBL
011	22	22	044	55	÷	077	12	B
012	75	-	045	53	(	078	43	RCL
013	43	RCL	046	43	RCL	079	27	27
014	23	23	047	24	24	080	33	X²
015	95	=	048	75	-	081	85	+
016	42	STO	049	43	RCL	082	01	1
017	26	26	050	23	23	083	95	=
018	43	RCL	051	54	)	084	34	√X
019	25	25	052	95	=	085	85	+
020	75	-	053	42	STO	086	01	1
021	43	RCL	054	27	27	087	85	+
022	26	26	055	53	(	088	43	RCL
023	95	=	056	43	RCL	089	27	27
024	55	÷	057	24	24	090	95	=
025	53	(	058	75	-	091	65	×
026	43	RCL	059	43	RCL	092	43	RCL
027	25	25	060	23	23	093	28	28
028	55	÷	061	54	)	094	94	+/-
029	43	RCL	062	55	÷	095	85	+
030	26	26	063	53	(	096	02	2
031	54	)	064	43	RCL	097	95	=
032	23	LNX	065	21	21	098	42	STO

(Continued) Table IV

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
099	30	30	143	85	+	187	76	LBL	231	33	X^2	275	23	LNX
100	43	RCL	144	01	1	188	13	C	232	85	+	276	42	STO
101	27	27	145	95	=	189	02	2	233	01	1	277	59	59
102	33	X^2	146	34	√X	190	55	÷	234	95	=	278	43	RCL
103	85	+	147	65	×	191	43	RCL	235	34	√X	279	27	27
104	01	1	148	43	RCL	192	28	28	236	42	STO	280	33	X^2
105	95	=	149	30	30	193	75	-	237	58	58	281	85	+
106	34	√X	150	95	=	194	01	1	238	85	+	282	01	1
107	94	+/-	151	42	STO	195	75	-	239	43	RCL	283	95	=
108	85	+	152	30	30	196	43	RCL	240	59	59	284	34	√X
109	01	1	153	43	RCL	197	27	27	241	95	=	285	65	×
110	85	+	154	27	27	198	95	=	242	55	÷	286	43	RCL
111	43	RCL	155	65	×	199	42	STO	243	53	(	287	59	59
112	27	27	156	43	RCL	200	30	30	244	43	RCL	288	55	÷
113	95	=	157	28	28	201	01	1	245	59	59	289	02	2
114	65	×	158	94	+/-	202	75	-	246	75	-	290	95	=
115	43	RCL	159	85	+	203	43	RCL	247	43	RCL	291	42	STO
116	28	28	160	01	1	204	27	27	248	58	58	292	59	59
117	94	+/-	161	95	=	205	65	×	249	54	)	293	43	RCL
118	85	+	162	35	1/X	206	43	RCL	250	95	=	294	27	27
119	02	2	163	65	×	207	28	28	251	23	LNX	295	75	-
120	95	=	164	53	(	208	95	=	252	35	1/X	296	01	1
121	55	÷	165	43	RCL	209	65	×	253	42	STO	297	95	=
122	43	RCL	166	28	28	210	53	(	254	30	30	298	35	1/X
123	30	30	167	94	+/-	211	01	1	255	01	1	299	65	×
124	95	=	168	85	+	212	75	-	256	75	-	300	43	RCL
125	23	LNX	169	01	1	213	43	RCL	257	43	RCL	301	59	59
126	42	STO	170	54	)	214	28	28	258	28	28	302	65	×
127	30	30	171	95	=	215	54	)	259	95	=	303	43	RCL
128	43	RCL	172	23	LNX	216	95	=	260	42	STO	304	30	30
129	27	27	173	65	×	217	34	√X	261	59	59	305	95	=
130	75	-	174	43	RCL	218	65	×	262	01	1	306	99	PRT
131	01	1	175	30	30	219	02	2	263	75	-	307	91	R/S
132	95	=	176	95	=	220	55	÷	264	43	RCL	308	65	×
133	65	×	177	99	PRT	221	43	RCL	265	27	27	309	43	RCL
134	43	RCL	178	91	R/S	222	28	28	266	65	×	310	29	29
135	30	30	179	65	×	223	85	+	267	43	RCL	311	95	=
136	95	=	180	43	RCL	224	43	RCL	268	28	28	312	42	STO
137	35	1/X	181	29	29	225	30	30	269	95	=	313	30	30
138	42	STO	182	95	=	226	95	=	270	35	1/X	314	99	PRT
139	30	30	183	42	STO	227	42	STO	271	65	×	315	91	R/S
140	43	RCL	184	30	30	228	59	59	272	43	RCL			
141	27	27	185	99	PRT	229	43	RCL	273	59	59			
142	33	X^2	186	91	R/S	230	27	27	274	95	=			

Listing for TI version—program B **Table V**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	014	93	.	028	65	×	042	01	01	056	76	LBL
001	11	A	015	01	1	029	53	(	043	65	×	057	22	INV
002	43	RCL	016	02	2	030	43	RCL	044	43	RCL	058	55	÷
003	10	10	017	65	×	031	24	24	045	06	06	059	43	RCL
004	55	÷	018	53	(	032	75	-	046	54	)	060	04	04
005	43	RCL	019	43	RCL	033	43	RCL	047	45	Y^X	061	55	÷
006	14	14	020	08	08	034	23	23	048	93	.	062	43	RCL
007	95	=	021	45	Y^X	035	54	)	049	08	8	063	05	05
008	45	Y^X	022	93	.	036	71	SBR	050	54	)	064	55	÷
009	93	.	023	06	6	037	22	INV	051	95	=	065	43	RCL
010	02	2	024	07	7	038	65	×	052	99	PRT	066	06	06
011	95	=	025	55	÷	039	53	(	053	44	SUM	067	92	RTN
012	65	×	026	43	RCL	040	53	(	054	33	33	068	76	LBL
013	01	1	027	30	30	041	43	RCL	055	91	R/S	069	12	B

(Continued) Table V

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
070	01	1	117	93	.	164	95	=	211	43	RCL	258	07	7
071	93	.	118	00	0	165	99	PRT	212	07	07	259	65	×
072	05	5	119	00	0	166	44	SUM	213	33	X^2	260	53	(
073	08	8	120	06	6	167	33	33	214	75	-	261	43	RCL
074	65	×	121	06	6	168	98	ADV	215	53	(	262	21	21
075	71	SBR	122	08	8	169	43	RCL	216	89	π	263	75	-
076	23	LNX	123	65	×	170	33	33	217	65	×	264	43	RCL
077	65	×	124	71	SBR	171	99	PRT	218	43	RCL	265	22	22
078	43	RCL	125	23	LNX	172	98	ADV	219	02	02	266	54	)
079	20	20	126	55	÷	173	91	R/S	220	33	X^2	267	55	÷
080	55	÷	127	43	RCL	174	76	LBL	221	54	)	268	43	RCL
081	43	RCL	128	18	18	175	15	E	222	95	=	269	30	30
082	01	01	129	71	SBR	176	32	X⇌T	223	55	÷	270	65	×
083	71	SBR	130	22	INV	177	00	0	224	89	π	271	53	(
084	22	INV	131	65	×	178	67	EQ	225	55	÷	272	53	(
085	95	=	132	53	(	179	24	CE	226	43	RCL	273	43	RCL
086	99	PRT	133	53	(	180	89	π	227	02	02	274	00	00
087	44	SUM	134	43	RCL	181	65	×	228	95	=	275	65	×
088	33	33	135	02	02	182	43	RCL	229	76	LBL	276	43	RCL
089	91	R/S	136	55	÷	183	02	02	230	32	X⇌T	277	03	03
090	76	LBL	137	43	RCL	184	33	X^2	231	45	Y^X	278	65	×
091	23	LNX	138	01	01	185	55	÷	232	93	.	279	43	RCL
092	43	RCL	139	54	)	186	04	4	233	04	4	280	09	09
093	10	10	140	23	LNX	187	95	=	234	05	5	281	55	÷
094	55	÷	141	54	)	188	94	+/-	235	65	×	282	43	RCL
095	43	RCL	142	95	=	189	85	+	236	93	.	283	07	07
096	14	14	143	99	PRT	190	43	RCL	237	01	1	284	55	÷
097	65	×	144	44	SUM	191	07	07	238	05	5	285	43	RCL
098	43	RCL	145	33	33	192	33	X^2	239	02	2	286	37	37
099	16	16	146	91	R/S	193	95	=	240	65	×	287	54	)
100	65	×	147	76	LBL	194	65	×	241	53	(	288	45	Y^X
101	43	RCL	148	14	D	195	04	4	242	43	RCL	289	93	.
102	08	08	149	01	1	196	55	÷	243	11	11	290	05	5
103	55	÷	150	93	.	197	89	π	244	55	÷	291	05	5
104	43	RCL	151	05	5	198	55	÷	245	43	RCL	292	54	)
105	30	30	152	08	8	199	43	RCL	246	15	15	293	95	=
106	65	×	153	65	×	200	02	02	247	54	)	294	71	SBR
107	53	(	154	71	SBR	201	95	=	248	45	Y^X	295	22	INV
108	43	RCL	155	23	LNX	202	61	GTO	249	93	.	296	95	=
109	24	24	156	65	×	203	32	X⇌T	250	04	4	297	99	PRT
110	75	-	157	43	RCL	204	76	LBL	251	05	5	298	44	SUM
111	43	RCL	158	19	19	205	24	CE	252	65	×	299	33	33
112	23	23	159	55	÷	206	03	3	253	43	RCL	300	98	ADV
113	54	)	160	43	RCL	207	93	.	254	38	38	301	43	RCL
114	92	RTN	161	02	02	208	04	4	255	45	Y^X	302	33	33
115	76	LBL	162	71	SBR	209	04	4	256	93	.	303	99	PRT
116	13	C	163	22	INV	210	65	×	257	06	6	304	98	ADV
												305	91	R/S

Listing for TI version—program C **Table VI**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	009	02	02	018	33	X^2	027	95	=	036	04	4
001	11	A	010	33	X^2	019	95	=	028	42	STO	037	04	4
002	32	X⇌T	011	55	÷	020	65	×	029	36	36	038	65	×
003	00	0	012	04	4	021	04	4	030	61	GTO	039	43	RCL
004	67	EQ	013	95	=	022	55	÷	031	23	LNX	040	07	07
005	22	INV	014	94	+/-	023	89	π	032	76	LBL	041	33	X^2
006	89	π	015	85	+	024	55	÷	033	22	INV	042	75	-
007	65	×	016	43	RCL	025	43	RCL	034	03	3	043	53	(
008	43	RCL	017	07	07	026	02	02	035	93	.	044	89	π

(Continued) Table VI

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
045	65	×	092	93	.	139	65	×	186	03	3	233	22	INV
046	43	RCL	093	00	0	140	01	1	187	02	2	234	52	EE
047	02	02	094	03	3	141	02	2	188	95	=	235	99	PRT
048	33	X^2	095	04	4	142	55	÷	189	35	1/X	236	32	X:T
049	54	)	096	04	4	143	43	RCL	190	65	×	237	91	R/S
050	95	=	097	95	=	144	13	13	191	93	.	238	55	÷
051	55	÷	098	45	Y^X	145	22	INV	192	01	1	239	32	X:T
052	89	π	099	93	.	146	52	EE	193	02	2	240	35	1/X
053	55	÷	100	01	1	147	95	=	194	05	5	241	85	+
054	43	RCL	101	09	9	148	99	PRT	195	85	+	242	53	(
055	02	02	102	06	6	149	98	ADV	196	93	.	243	93	.
056	95	=	103	04	4	150	91	R/S	197	00	0	244	00	0
057	42	STO	104	94	+/-	151	76	LBL	198	00	0	245	02	2
058	36	36	105	95	=	152	13	C	199	01	1	246	07	7
059	76	LBL	106	65	×	153	43	RCL	200	04	4	247	65	×
060	23	LNX	107	93	.	154	10	10	201	95	=	248	43	RCL
061	43	RCL	108	00	0	155	65	×	202	65	×	249	05	05
062	11	11	109	01	1	156	01	1	203	93	.	250	55	÷
063	65	×	110	02	2	157	08	8	204	00	0	251	43	RCL
064	43	RCL	111	08	8	158	03	3	205	02	2	252	12	12
065	07	07	112	65	×	159	55	÷	206	08	8	253	65	×
066	65	×	113	43	RCL	160	43	RCL	207	02	2	254	53	(
067	43	RCL	114	57	57	161	01	01	208	65	×	255	43	RCL
068	37	37	115	33	X^2	162	33	X^2	209	43	RCL	256	56	56
069	65	×	116	65	×	163	55	÷	210	56	56	257	55	÷
070	01	1	117	43	RCL	164	43	RCL	211	33	X^2	258	43	RCL
071	04	4	118	04	04	165	06	06	212	65	×	259	12	12
072	04	4	119	65	×	166	95	=	213	43	RCL	260	65	×
073	55	÷	120	43	RCL	167	42	STO	214	04	04	261	04	4
074	43	RCL	121	37	37	168	56	56	215	65	×	262	93	.
075	03	03	122	55	÷	169	65	×	216	43	RCL	263	04	4
076	55	÷	123	43	RCL	170	43	RCL	217	05	05	264	05	5
077	43	RCL	124	00	00	171	01	01	218	55	÷	265	52	EE
078	09	09	125	65	×	172	55	÷	219	05	5	266	94	+/-
079	55	÷	126	43	RCL	173	02	2	220	93	.	267	06	6
080	43	RCL	127	03	03	174	93	.	221	02	2	268	54	)
081	00	00	128	55	÷	175	04	4	222	02	2	269	33	X^2
082	95	=	129	05	5	176	02	2	223	52	EE	270	54	)
083	42	STO	130	93	.	177	55	÷	224	01	1	271	95	=
084	57	57	131	02	2	178	01	1	225	00	0	272	22	INV
085	65	×	132	02	2	179	02	2	226	55	÷	273	52	EE
086	43	RCL	133	52	EE	180	55	÷	227	43	RCL	274	99	PRT
087	36	36	134	01	1	181	43	RCL	228	01	01	275	98	ADV
088	55	÷	135	00	0	182	14	14	229	65	×	276	91	R/S
089	43	RCL	136	55	÷	183	95	=	230	01	1			
090	15	15	137	43	RCL	184	45	Y^X	231	02	2			
091	65	×	138	36	36	185	93	.	232	95	=			

User instructions for TI version **Table VII**

The TI version is in three parts, and must be run in order. However, all the data may be stored before any one of the parts is run, but not all the parts use all the data. The following tabulation shows the data storage areas and the data used by the separate programs.

(Note: The HP version calls for entering data between operation of the different parts of the program. This is because some of the HP storage areas are used for more than one value. The TI calculator has more storage capacity than the HP, so that all of the data may be entered before the start of program A, inasmuch as none of the storage areas are used for more than one value.)

Data	Register	Program Use A	Program Use B	Program Use C
Baffle spacing, in.	00		*	*
Tube I.D., in.	01		*	*
Tube O.D., in.	02		*	*

(Continued) Table VII

Shell diameter, in.	03		*	*
Tube length, in.	04		*	*
No. of tube passes	05		*	*
No. tubes per pass	05		*	*
Tube pitch, in.	07		*	*
Prandtl number, inside	08		*	
Prandtl number, outside	38		*	
Tube clearance	09		*	*
Weight flowrate, cold fluid, lb/h	10		*	*
Weight flowrate, hot fluid, lb/h	11		*	*
Specific gravity, cold fluid	12			*
Specific gravity, hot fluid	13			*
Viscosity, cold fluid, cP	14		*	*
Viscosity, hot fluid, cP	15		*	*
Thermal conductivity, cold	16		*	
Thermal conductivity, hot	17			
Thermal conductivity, tube	18		*	
Fouling factor, outside	19		*	
Fouling factor, inside	20		*	
Temperatures, °F				
Hot fluid, inlet	21	*	*	
Hot fluid, outlet	22	*	*	
Cold fluid, inlet	23	*	*	
Cold fluid, outlet	24	*	*	
Number of passes	37		*	*

Programs are run as follows:

Part A: Key **A** gives LMTD.
Key **B** gives $F_{T,1-2}$ (if result is flashing, it indicates a temperature cross and inoperable condition. Use key **CLR**.)
Key **C** gives $F_{T,2-4}$.
Key **R/S** gives corrected LMTD for F_T.

Part B: Keys **A, B, C, D, E** give fractional temperature drops indicated in Table II.
After key **D,** program prints both the *D* fraction (R_D) and the sum.
Before key **E,** enter "0" for triangular tube array or "1" or square tube array.
After key **E,** programs prints both the *E* fraction and the sum.

Part C: Enter "0" for triangular tube array or "1" for square tube array.
Press key **A**
Output will be shell-side pressure drop, psi.
Press key **C**
When program stops, enter ϕ + 0.14 and key **R/S.**
Output will be tube-side pressure drop, psi.

Printout for first example—TI Version **Table VII**

Program A

```
 71.9314240
.9585302826
0.924290356
66.48552224
```

Program B

```
 0.09534324
          0.
.0034283053
.2954729306

.3842444759

.5393019662

.9235464421
```

Program C

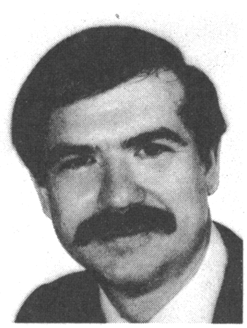
```
6.205625639

3.386938169
6.403467672
```

References

1. Standards of Tubular Exchanger Manufacturers Assn. (TEMA), Sixth ed., New York, 1978.
2. Kern, D. Q., "Process Heat Transfer," McGraw-Hill Book Co., New York, 1950.
3. Gilmour, C. H., "Shortcut to heat exchanger design—I," *Chem. Eng.*, Oct. 1952.

The authors



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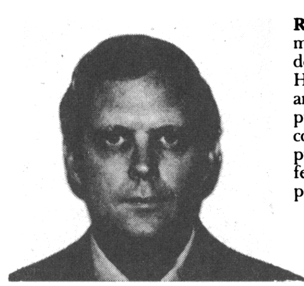

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Section VI
Mass Transfer

Shortcut program for multicomponent distillation

This TI-59 program calculates the minimum reflux, minimum number of stages, and number of theoretical stages for a multicomponent distillation column.

Mark Kesler, *Kesler Engineering, Inc.*

☐ A rough distillation-column design speeds up scoping studies, preliminary cost estimates, and parametric evaluations of operating variables. When great accuracy is not needed, the shortcut method is preferred to rigorous design procedures because it saves time and money.

The most widely accepted shortcut method for multicomponent distillation columns uses the Underwood equations for minimum reflux, the Fenske equations for minimum stages, and the Gilliland correlations for the number of stages for a given reflux. With these results in hand, the engineer then determines tray hydraulics and efficiencies, and sizes the column.

Because even the shortcut is time-consuming when calculated by hand, it pays to use this TI-59 program. The program calculates the minimum reflux, minimum number of stages, and number of theoretical stages for any one-feed column distilling eight or fewer components. The required inputs are feed, overhead and bottoms compositions; feed condition; and relative volatilities for all components.

Key assumptions

The shortcut method and the calculator program are based on several assumptions:

- There is only one feed stream, with eight or fewer components.
- There is only one heavy key component.
- The feed enters the column at the optimal stage.
- The correlation assumes constant molar overflows.

Developing the inputs

Column design usually begins with the following information: feed composition, feed temperature, and desired separation. Before using the program, one must collect more data and perform a few calculations:

1. Calculate the material balance for the column. The feed, overhead and bottoms compositions (mole fractions) are inputs to the program.
2. Set the relative volatility (α) for the heavy key component equal to 1. Then determine the α values for the other components relative to the heavy key. The α values can be based on the feed temperature, but average α values (for feed, overhead and bottoms temperatures) are more accurate:

$$\alpha_i = (\alpha_{overhead} \cdot \alpha_{feed} \cdot \alpha_{bottoms})_i^{1/3}$$

Note: The program will not work if α for the heavy key is not equal to 1.

3. Determine the liquid mole fraction (q) of the feed. A bubble-point feed has $q = 1.0$; a dewpoint feed has $q = 0$.
4. Rank the components in order of decreasing relative volatility (α). Thus, component 1 will be the most volatile component. List all of the inputs in a table.

Example: Table I shows the input data required to calculate R_{min} and N_{min} for a simplified debutanizer column. Note that i-C_5 is the heavy key component (with $\alpha = 1$) and that all of the components are arranged in order of decreasing α.

How the program works

After all of the input data are stored in the memories, the program first finds the heavy key component. The program looks for $\alpha_i = 1$, then designates component i as the heavy key and component $i - 1$ as the light key.

Inputs for debutanizer example; i-C_5 is the heavy key — Table I

Component	i	Feed (F_i)	Overhead (D_i)	Bottoms (B_i)	Relative volatility (α_i)
C_3	1	0.05	0.102	0.000	4.99
i-C_4	2	0.15	0.301	0.004	2.62
n-C_4	3	0.25	0.473	0.033	2.02
i-C_5	4	0.20	0.069	0.327	1.00
n-C_5	5	0.35	0.055	0.636	0.86
		1.00	1.000	1.000	

q=1.0 (bubble-point feed)

Originally published May 4, 1981.

Program listing for TI-59 calculator **Table II**

Location	Code	Key
Find heavy key		
000	76	LBL
001	17	B'
002	43	RCL
003	40	40
004	42	STO
005	01	01
006	42	STO
007	19	19
008	42	STO
009	20	20
010	76	LBL
011	52	EE
012	02	2
013	00	0
014	85	+
015	43	RCL
016	01	01
017	95	=
018	42	STO
019	35	35
020	01	1
021	32	X:T
022	43	RCL
023	01	01
024	75	-
025	01	1
026	95	=
027	42	STO
028	01	01
029	73	RC*
030	35	35
031	22	INV
032	77	GE
033	52	EE
034	43	RCL
035	01	01
036	85	+
037	02	2
038	00	0
039	95	=
040	42	STO
041	35	35
042	73	RC*
043	35	35
044	42	STO
045	33	33
046	00	0
047	42	STO
048	01	01
049	61	GTO
050	01	01
051	26	26
Calculate θ		
052	76	LBL
053	16	A'
054	42	STO
055	10	10
056	43	RCL
057	19	19
058	42	STO
059	40	40
060	00	0
061	42	STO
062	32	32
063	29	CP
064	76	LBL
065	23	LNX
066	53	(
067	02	2
068	00	0
069	85	+
070	43	RCL
071	40	40
072	54	)
073	42	STO
074	35	35
075	53	(
076	01	1
077	00	0
078	85	+
079	43	RCL
080	40	40
081	54	)
082	42	STO
083	31	31
084	53	(
085	73	RC*
086	35	35
087	65	×
088	73	RC*
089	31	31
090	55	÷
091	53	(
092	73	RC*
093	35	35
094	75	-
095	43	RCL
096	10	10
097	54	)
098	54	)
099	44	SUM
100	32	32
101	53	(
102	43	RCL
103	40	40
104	75	-
105	01	1
106	54	)
107	42	STO
108	40	40
109	22	INV
110	67	EQ
111	23	LNX
112	53	(
113	43	RCL
114	32	32
115	85	+
116	43	RCL
117	50	50
118	75	-
119	01	1
120	54	)
121	42	STO
122	34	34
123	43	RCL
124	34	34
125	92	RTN
126	01	1
127	93	.
128	00	0
129	00	0
130	00	0
131	05	5
132	36	PGM
133	08	08
134	11	A
135	43	RCL
136	33	33
137	36	PGM
138	08	08
139	12	B
140	93	.
141	01	1
142	36	PGM
143	08	08
144	13	C
145	93	.
146	00	0
147	00	0
148	01	1
149	36	PGM
150	08	08
151	14	D
152	36	PGM
153	08	08
154	15	E
155	00	0
Calculate R_{min}		
156	42	STO
157	37	37
158	76	LBL
159	33	X^2
160	29	CP
161	05	5
162	00	0
163	85	+
164	43	RCL
165	19	19
166	95	=
167	42	STO
168	35	35
169	02	2
170	00	0
171	85	+
172	43	RCL
173	19	19
174	95	=
175	42	STO
176	36	36
177	73	RC*
178	35	35
179	65	×
180	73	RC*
181	36	36
182	55	÷
183	53	(
184	73	RC*
185	36	36
186	75	-
187	43	RCL
188	10	10
189	54	)
190	95	=
191	44	SUM
192	37	37
193	43	RCL
194	19	19
195	75	-
196	01	1
197	95	=
198	42	STO
199	19	19
200	22	INV
201	67	EQ
202	33	X^2
203	43	RCL
204	37	37
205	75	-
206	01	1
207	95	=
208	42	STO
209	29	29
210	91	R/S
Calculate N_{min}		
211	76	LBL
212	18	C'
213	02	2
214	00	0
215	85	+
216	43	RCL
217	20	20
218	95	=
219	42	STO
220	35	35
221	01	1
222	32	X:T
223	43	RCL
224	20	20
225	75	-
226	01	1
227	95	=
228	42	STO
229	20	20
230	73	RC*
231	35	35
232	22	INV
233	77	GE
234	18	C'
235	43	RCL
236	20	20
237	85	+
238	05	5
239	01	1
240	95	=
241	42	STO
242	35	35
243	75	-
244	01	1
245	95	=
246	42	STO
247	31	31
248	43	RCL
249	20	20
250	85	+
251	04	4
252	00	0
253	95	=
254	42	STO
255	38	38
256	85	+
257	01	1
258	95	=
259	42	STO
260	39	39
261	73	RC*
262	31	31
263	65	×
264	73	RC*
265	39	39
266	55	÷
267	73	RC*
268	35	35
269	55	÷
270	73	RC*
271	38	38
272	95	=
273	28	LOG
274	55	÷
275	43	RCL
276	33	33
277	28	LOG
278	95	=
279	42	STO
280	49	49
281	91	R/S
Subroutine to calculate missing one of N, R, N_{min}, R_{min}		
282	76	LBL
283	19	D'
284	29	CP
285	43	RCL
286	29	29
287	42	STO
288	01	01
289	43	RCL
290	49	49
291	42	STO
292	03	03
293	76	LBL
294	44	SUM
295	43	RCL
296	01	01
297	22	INV
298	67	EQ
299	34	$\sqrt{x}$
300	71	SBR
301	28	LOG
302	61	GTO
303	39	COS
304	76	LBL
305	28	LOG
306	43	RCL
307	04	04
308	75	-
309	43	RCL
310	03	03
311	95	=
312	55	÷
313	53	(
314	43	RCL
315	04	04
316	85	+
317	01	1
318	54	)
319	95	=
320	42	STO
321	05	05
322	53	(
323	01	1
324	75	-
325	01	1
326	93	.
327	03	3
328	03	3
329	03	3
330	65	×
331	43	RCL
332	05	05
333	54	)
334	45	Y^X
335	01	1
336	93	.
337	07	7
338	06	6
339	04	4
340	03	3
341	95	=
342	42	STO
343	06	06
344	92	RTN
345	76	LBL
346	39	COS
347	43	RCL
348	06	06
349	65	×
350	53	(
351	43	RCL
352	02	02
353	85	+
354	01	1
355	54	)
356	95	=
357	94	+/-
358	85	+
359	43	RCL
360	02	02
361	95	=
362	91	R/S
363	76	LBL
364	34	$\sqrt{x}$

Table II (continued)

Location	Code	Key	Location	Code	Key
365	43	RCL	427	05	5
366	02	02	428	94	+/-
367	22	INV	429	85	+
368	67	EQ	430	93	.
369	35	1/X	431	07	7
370	71	SBR	432	05	5
371	28	LOG	433	95	=
372	53	(	434	42	STO
373	43	RCL	435	08	08
374	01	01	436	92	RTN
375	85	+	437	76	LBL
376	43	RCL	438	38	SIN
377	06	06	439	43	RCL
378	54	)	440	08	08
379	55	÷	441	65	×
380	53	(	442	53	(
381	01	1	443	43	RCL
382	75	-	444	04	04
383	43	RCL	445	85	+
384	06	06	446	01	1
385	54	)	447	54	)
386	95	=	448	95	=
387	91	R/S	449	94	+/-
388	76	LBL	450	85	+
389	35	1/X	451	43	RCL
390	43	RCL	452	04	04
391	03	03	453	95	=
392	22	INV	454	91	R/S
393	67	EQ	455	76	LBL
394	24	CE	456	24	CE
395	71	SBR	457	71	SBR
396	25	CLR	458	25	CLR
397	61	GTO	459	43	RCL
398	38	SIN	460	03	03
399	76	LBL	461	85	+
400	25	CLR	462	43	RCL
401	43	RCL	463	08	08
402	02	02	464	95	=
403	75	-	465	94	+/-
404	43	RCL	466	55	÷
405	01	01	467	53	(
406	95	=	468	43	RCL
407	55	÷	469	08	08
408	53	(	470	75	-
409	43	RCL	471	01	1
410	02	02	472	54	)
411	85	+	473	95	=
412	01	1	474	91	R/S
413	54	)			
414	95	=			
415	42	STO			
416	07	07			
417	45	Y^X			
418	93	.			
419	05	5			
420	06	6			
421	06	6			
422	08	8			
423	95	=			
424	65	×			
425	93	.			
426	07	7			

Nomenclature

- B_i Mole fraction of component i in bottoms
- D_i Mole fraction of component i in overhead
- F_i Mole fraction of component i in feed
- k Number of components in feed ($k \leq 8$)
- N Number of theoretical stages
- N_{min} Minimum number of theoretical stages
- q Liquid mole fraction in feed (0.0 for dewpoint; 1.0 for bubble point)
- R Reflux ratio
- R_{min} Minimum reflux ratio
- α_i Relative volatility of component i, based on heavy key ($\alpha = 1$ for heavy key component)
- θ Variable in Underwood correlation

Again, it is essential that the components be arranged in order of decreasing α, and that the heavy key component have $\alpha = 1$.

The program then uses the Underwood correlation [*1*] to find the minimum reflux ratio (R_{min}). The equation is:

$$R_{min} = \left(\sum_{1}^{k} \frac{\alpha_i D_i}{\alpha_i - \theta}\right) - 1$$

where k is the number of components, and θ is determined by trial and error, using the following equation:

$$1 - q = \sum_{1}^{k} \frac{\alpha_i F_i}{\alpha_i - \theta}$$

The Underwood correlation requires that the overhead composition be consistent with minimum reflux conditions. But this program uses actual overhead compositions: this is simpler, and nearly as accurate.

After finding R_{min}, the program calculates the minimum number of stages (N_{min}), using the Fenske equation [*2*]:

$$N_{min} = \log\left[\frac{D_{lk}B_{hk}}{D_{hk}B_{lk}}\right]\left(\frac{1}{\log \alpha_{lk}}\right)$$

where the subscripts hk and lk denote the heavy and light key components.

The user then determines the desired reflux ratio (R) based on R_{min}. With this additional input, the program will calculate the number of theoretical stages (N), using the Gilliland correlation [*3*] as expressed by Eduljee [*4*]:

$$\frac{N - N_{min}}{N + 1} = 0.75 - 0.75\left(\frac{R - R_{min}}{R + 1}\right)^{0.5668}$$

Alternatively, the user can input the desired value of N, and the program can find R, using the equation above.

How to use the program

Prepare all of the required input data as shown in Table I. Load the program, listed in Table II, into the calculator. Then follow the user instructions in Table III. The Master Library Module must be in place for the program to work.

User instructions **Table III**

Step	Description	Enter	Press	Display
1	Input feed composition (up to eight components) in order of decreasing volatility	$F_1, F_2 \ldots$	STO 11, STO 12...	$F_1, F_2 \ldots$
2	Input relative volatility (α must be 1.0 for heavy key)	$\alpha_1, \alpha_2 \ldots$	STO 21, STO 22 ...	$\alpha_1, \alpha_2 \ldots$
3	Input bottoms composition	$B_1, B_2 \ldots$	STO 41, STO 42...	$B_1, B_2 \ldots$
4	Input overhead composition	$D_1, D_2 \ldots$	STO 51, STO 52...	$D_1, D_2 \ldots$
5	Input number of components ($k \leqslant 8$)	k	STO 40	k
6	Input feed condition (q=0 for dew point; q=1 for bubble point)	q	STO 50	q
7	Calculate minimum reflux ratio (run time 3-5 min)		2nd **B′**	R_{min}
8	Calculate minimum number of stages		2nd **C′**	N_{min}
9	Input desired reflux ratio ($R > R_{min}$)	R	STO 2	R
10	Calculate number of stages		2nd **D′**	N

Notes:
To calculate R_{min} and N_{min} for new conditions, change the inputs as needed and return to step 7.
Given any three of the four variables R_{min}, N_{min}, R and N in memory, pressing 2nd **D′** will calculate the fourth.

Data registers used in program **Table IV**

00 Not used	20 Number of components (k)	40 Number of components (k)
01 R_{min}	21 α_i values	41 B_i values
02 R	22 "	42 "
03 N_{min}	23 "	43 "
04 N	24 "	44 "
05 Used	25 "	45 "
06 "	26 "	46 "
07 "	27 "	47 "
08 "	28 "	48 "
09 "	29 R_{min}	49 N_{min}
10 Θ	30 Used	50 Feed condition (q)
11 F_i values	31 Loop counter	51 D_i values
12 "	32 Used	52 "
13 "	33 D_{lk}	53 "
14 "	34 $1-q$	54 "
15 "	35 Used	55 "
16 "	36 Loop counter	56 "
17 "	37 Used	57 "
18 "	38 Loop counter	58 "
19 Number of components (k)	39 "	59 Not used

In the program listing in Table II, several of the listed keystrokes are not keystrokes at all, but instead are display conventions used by the TI-59 calculator.

To be able to key in the program, make the following changes:

1. Wherever **RC*** appears, substitute **RCL 2nd Ind.**
2. Wherever **RTN** appears, substitute **INV SBR.**

RC* appears in steps 029, 042, 085, 088, 092, 177, 180, 184, 230, 261, 264, 267 and 270. **RTN** appears in steps 125, 344, and 436.

The displays **RC*** and **RTN** will appear again when the program is listed. The "Personal Programming" book explains these displays.

Note that the program includes a subroutine labeled **D′** that can calculate one of the values N, N_{min}, R or R_{min}, when the other three values are stored in the proper registers. Table IV shows the contents of the data registers used in the program.

Example: Find R_{min} and N_{min} for the data given in Table I. First, key in the data as shown in the user instructions. To find R_{min}, press **B′**, wait 3–5 min, and read the value of R_{min} when it appears in the display:

$$R_{min} = .9351686744$$

Then press **C′** to find N_{min} (instant):

$$N_{min} = 5.999795796$$

Enter the actual value of R desired. For instance, to specify a reflux ratio 25% greater than the minimum, multiply R_{min} by 1.25 to get R:

$$R = 1.168960843$$

Store R in register 2, and press **D′** to find N:

$$N = 14.14481751$$

Thus, the number of theoretical stages is about 14 for a reflux ratio 25% greater than the minimum, compared to six stages for minimum reflux ratio.

For HP-67/97 users

The HP version closely follows the TI program. Table V is a listing of the HP program, and user instructions are presented in Table VI.

The calculation of Θ, the variable in the Underwood equation, takes about 4 minutes. This variable is not printed; it is only displayed. Also, values calculated by the HP will differ slightly from those calculated by the TI. This difference is probably because the TI calculates Θ to an error of 0.005 and the HP calculates it to an error of 0.0001. The difference in calculated values is not significant to two decimals. An example of such a difference is the calculation of R_{min}. The TI value is 0.935168 . . . and the HP value is 0.937266. . . .

Program listing for HP version **Table V**

Step	Key	Code	Step	Key	Code
010	1	01	065	*LBL7	21 07
011	STOC	35 13	066	RCLA	36 11
012	*LBLa	21 16 11	067	1	01
013	1	01	068	RCLC	36 13
014	STOI	35 46	069	+	-55
015	*LBL1	21 01	070	÷	-24
016	RCLi	36 45	071	STOA	35 11
017	P⇄S	16-51	072	RCLC	36 13
018	RCLi	36 45	073	1	01
019	×	-35	074	0	00
020	RCLi	36 45	075	÷	-24
021	RCLA	36 11	076	STOC	35 13
022	-	-45	077	GTO9	22 09
023	÷	-24	078	*LBL6	21 06
024	ST+9	35-55 09	079	SF0	16 21 00
025	ISZI	16 26 46	080	RCL9	36 09
026	P⇄S	16-51	081	STOB	35 12
027	RCL0	36 00	082	*LBL9	21 09
028	RCLI	36 46	083	RCLA	36 11
029	X>Y?	16-34	084	1	01
030	GTO2	22 02	085	RCLC	36 13
031	GTO1	22 01	086	+	-55
032	*LBL2	21 02	087	×	-35
033	P⇄S	16-51	088	STOA	35 11
034	RCL9	36 09	089	0	00
035	1	01	090	STO9	35 09
036	RCL0	36 00	091	P⇄S	16-51
037	-	-45	092	GTOa	22 16 11
038	-	-45	093	*LBL2	21 02
039	ABS	16 31	094	P⇄S	16-51
040	.	-62	095	R/S	51
041	0	00	096	1	01
042	0	00	097	STOI	35 46
043	0	00	098	*LBLb	21 16 12
044	1	01	099	RCLi	36 45
045	X>Y?	16-34	100	P⇄S	16-51
046	GTO2	22 02	101	RCLi	36 45
047	F0?	16 23 00	102	×	-35
048	GTO5	22 05	103	1	01
049	GTO6	22 06	104	RCLi	36 45
050	*LBL5	21 05	105	X≠Y?	16-32
051	0	00	106	GTO2	22 02
052	RCL9	36 09	107	RCLI	36 46
053	X>Y?	16-34	108	STOB	35 12
054	GTO5	22 05	109	R↓	-31
055	R↓	-31	110	*LBL2	21 02
056	RCLB	36 12	111	R↓	-31
057	X>Y?	16-34	112	R↓	-31
058	GTO7	22 07	113	RCLi	36 45
059	GTO6	22 06	114	RCLA	36 11
060	*LBL5	21 05	115	-	-45
061	R↓	-31	116	÷	-24
062	RCLB	36 12	117	P⇄S	16-51
063	X>Y?	16-34	118	ST+9	35-55 09
064	GTO6	22 06	119	ISZI	16 26 46

(Continued) Table V

Step	Key	Code	Step	Key	Code
120	RCL0	36 00	172	Y^x	31
121	RCLI	36 46	173	.	-62
122	X>Y?	16-34	174	7	07
123	GTO2	22 02	175	5	05
124	GTOb	22 16 12	176	×	-35
125	*LBL2	21 02	177	CHS	-22
126	1	01	178	.	-62
127	ST-9	35-45 09	179	7	07
128	RCLB	36 12	180	5	05
129	STOI	35 46	181	+	-55
130	RCLi	36 45	182	STOD	35 14
131	DSZI	16 25 46	183	RCLB	36 12
132	RCLi	36 45	184	STOC	35 13
133	X⇄Y	-41	185	*LBLE	21 15
134	÷	-24	186	RCLC	36 13
135	STOC	35 13	187	RCLD	36 14
136	R/S	51	188	+	-55
137	RCLi	36 45	189	1	01
138	ISZI	16 26 46	190	RCLD	36 14
139	RCLi	36 45	191	-	-45
140	X⇄Y	-41	192	÷	-24
141	÷	-24	193	PRTX	-14
142	RCLC	36 13	194	R/S	51
143	×	-35	195	*LBLd	21 16 14
144	LN	32	196	STOA	35 11
145	P⇄S	16-51	197	RCLB	36 12
146	DSZI	16 25 46	198	-	-45
147	RCLi	36 45	199	RCLA	36 11
148	LN	32	200	1	01
149	÷	-24	201	+	-55
150	STOB	35 12	202	÷	-24
151	P⇄S	16-51	203	.	-62
152	RCL9	36 09	204	7	07
153	PRTX	-14	205	5	05
154	RCLB	36 12	206	-	-45
155	PRTX	-14	207	.	-62
156	CF0	16 22 00	208	7	07
157	SPC	16-11	209	5	05
158	R/S	51	210	CHS	-22
159	*LBLD	21 14	211	÷	-24
160	STOA	35 11	212	.	-62
161	RCL9	36 09	213	5	05
162	-	-45	214	6	06
163	RCLA	36 11	215	6	06
164	1	01	216	8	08
165	+	-55	217	1/X	52
166	÷	-24	218	Y^x	31
167	.	-62	219	STOD	35 14
168	5	05	220	RCL9	36 09
169	6	06	221	STOC	35 13
170	6	06	222	GTOE	22 15
171	8	08	223	R/S	51

User instructions for HP version **Table VI**

Store the following data:

Number of components, *k* (maximum 8)	**STO 0**
Fraction of component in feed, F_i	**STO 1 to k**
Switch storage areas	key **P ⇄ S**
Fraction liquid in feed, *q*	**STO 0**
Relative volatilities, α_i	**STO 1 to k**
Switch storage areas	key **P ⇄ S**

(Continued) Table VI

Key **A**	
Program then calculates Θ, variable in Underwood correlation. Calculation may take a few minutes.	
Then, store overhead data, D_i	**STO 1 to k**
Key **R/S**	
Then, store bottoms data, B_i	**STO 1 to k**
Key **R/S**	
Output will be: Minimum reflux, R_{min} Minimum theoretical stages, N_{min}	
Input actual reflux R Output will be actual number of stages, N	key **D**
Input actual number of stages N, Output will be actual reflux ratio, R	key **d**

Note: Data cannot all be stored before the program is started, as in the TI version, because the HP-67/97 has limited storage capacity.

References

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Program aids cryogenic solubility calculations

Here is a program that will quickly estimate and correlate the solubility of a solid in a solvent at cryogenic temperatures.

Patrice Lebrun, *Chemical Engineer*

☐ In the design of cryogenic processes, it is frequently necessary to check the solubility of solids in liquids at low temperatures. The interest in predicting such behavior is justified because precipitation of solids such as carbon dioxide and hydrocarbons creates solid coatings on heat exchangers and fouling in process equipment.

This blocking effect can be prevented by appropriate design and a good knowledge of solubility. Unfortunately, two factors limit our precise information on solubility:

1. Solubility exhibits a very broad range of variation; for example, from 10^{-2} to 10^{-3} for light alkanes in nitrogen, to 10^{-10} for ammonia in nitrogen at 77 K.
2. In experimental investigations, there are sometimes great discrepancies between the findings of different authors (for example, as much as a factor of 60 for the system propylene-nitrogen).

Reliable experimental studies of solubility are not plentiful, and therefore it is desirable to have correlations that are sufficiently accurate for most design purposes. One of the best known of these correlations is that of Preston and Prausnitz [*1*], and that is the one used here.

The program presented in this article is intended to provide a quick estimate of solubility. It is written for the Hewlett-Packard HP 67/97 and features a rapidly converging iterative procedure. The program circumvents the use of tedious charts and laborious hand-calculations.

The Preston/Prausnitz method

These authors worked out a method of calculating the molar solubility, X_2, of a solid in cryogenic liquids, based on the Scatchard-Hildebrand concept for regular solutions [*2*].

In the solid-liquid equilibrium, where the solid phase is pure solute and the liquid phase is a saturated solution of the solute in the solvent, the equation of equilibrium is:

$$f_2^S = \gamma_2 X_2 f_2^L \quad (1)$$

$$\ln \gamma_2 X_2 = \Delta S_{F2}/R(1 - T_{M2}/T) \quad (2)$$

Some substances undergo solid-phase transitions from one crystal structure to another at a specific temperature, T_{TR}. If the solute of interest undergoes such a transition, and if T is less than T_{TR}, another term must be added to Eq. (2):

$$\ln \gamma_2 X_2 = (\Delta S_{F2}/R)(1 - T_{M2}/T) + (\Delta S_{TR}/R)(1 - T_{TR}/T) \quad (3)$$

The activity coefficient for conditions not near the critical temperature of the solvent is calculated by the relationship:

$$\ln \gamma_2 = (V_2\phi_1^2/RT)[(\delta_1 - \delta_2)^2 + 2\ell_{1,2}\delta_1\delta_2] \quad (4)$$

where

$$\phi_1 = X_1V_1/(X_1V_1 + X_2V_2) \quad (5)$$

The solubility X_2 of solute 2 in solvent 1 is determined by combining Eq. (2) or (3) with Eq. (4) and (5). Since X_2 and ϕ_1 are unknown, the calculation is done by trial and error.

An essential step in calculating solid solubility is finding the solubility parameter, δ, and the subcooled liquid volume, V, for solute and solvent. These properties are functions of the reduced properties T_r, P_r and of the acentric factor ω [*1*]. The relationships were determined via data-correlating programs, and the results are shown in Table I.

$\ell_{1,2}$ is a constant characteristic of the solute-solvent pair and it cannot be estimated from pure component data (see Table II). Hence:

1. When possible, $\ell_{1,2}$ should be determined empirically from some experimental equilibrium (see Example 3).
2. If no solid-phase information is available, we can turn to gas-phase data. It is known that for mixtures in the gas phase, the binary parameter, $k_{1,2}$, characterizes

(Text continues on p. 202)

Curve fitting of Ref. [*1*] — **Table I**

For $T_r < 0.7$

$$\delta/P_C^{1/2} = \{\omega[3.339\omega - 2.04] - 0.6312\}T_r^2 + 1.2165 + \omega[1.82 - 1.345\omega]$$

$$V/V_C = \{0.1452 + \omega[0.196 - 0.169\omega]\}T_r^2 + 0.339 - 0.15\omega$$

Originally published July 13, 1981.

Pure component properties **Table II**

Substance		P_C	T_C	V_C	ω	T_F	$\Delta S_F/R$	T_{TR}	$\Delta S_{TR}/R$
Nitrogen	N_2	33.5	126.2	90	0.040	63.2	1.37	35.5	0.78
Methane	CH_4	45.8	191.1	99	0.013	90.7	1.25	20.4	0.45
Ethane	C_2H_6	48.3	305.6	148	0.105	89.9	3.82		
Propane	C_3H_8	42.0	370.0	200	0.152	85.5	4.96		
Butane	C_4H_{10}	37.5	425.2	255	0.201	134.8	4.16	107.6	2.31
Isobutane	C_4H_{10}	36.0	408.1	263	0.192	113.7	4.80		
2-Methylbutane (Isopentane)	C_5H_{12}	32.9	461.0	308	0.206	113.2	5.47		
Pentane	C_5H_{12}	33.3	469.8	311	0.252	143.4	7.04		
2.2-Dimethylpropane (Neopentane)	C_5H_{12}	31.6	433.8	303	0.195	456.6	1.53		
Hexane	C_6H_{14}	29.9	507.9	368	0.290	177.8	8.81		
Heptane	C_7H_{16}	27.0	540.3	426	0.352	182.5	9.24		
Octane	C_5H_{18}	24.6	568.6	486	0.408	216.4	11.53		
Nonane	C_9H_{20}	22.6	596.2	543	0.441	219.6	8.47	217.2	3.48
Decane	$C_{10}H_{22}$	20.8	617.6	602	0.486	243.5	14.18		
Ethylene	C_2H_4	50.5	283.1	124	0.087	104.0	3.88		
Propene (Propylene)	C_3H_6	45.4	365.1	181	0.143	87.9	4.11		
Butene-1 (Butylene)	C_4H_8	38.7	419.5	241	0.203	87.8	5.27		
2-Methylpropane (Isobutene)	C_4H_8	39.5	417.8	240	0.201	132.8	5.36		
Pentene-1	C_5H_{10}	40.4	475.5	309	0.238	107.8	5.50		
Pentene-2 (cis)	C_5H_{10}	34.4	473.1	300	0.280	94.1	9.09		
Hexene-1	C_6H_{12}	31.1	504.0	356	0.283	133.3	8.43		
Heptene-1	C_7H_{14}	27.4	537.2	418	0.326	154.1	9.87		
Acetylene	C_2H_2	61.7	308.7	113	0.186	192.4	2.55		
Benzene	C_6H_6	48.6	562.6	260	0.215	278.7	4.25		
Toluene	C_7H_8	40.0	594.0	320	0.233	178.2	4.47		
p-Xylene	C_8H_{10}	33.9	618.8	378	0.293	286.4	7.19		
Cyclohexane	C_6H_{12}	40.0	553.2	308	0.211	279.7	1.15	186.1	4.36
Methylcyclohexane	C_7H_{14}	34.3	572.1	344	0.237	146.6	5.54		
Hydrogen sulfide	H_2S	88.9	373.6	97.7	0.100	187.6	1.52	103.5	1.79
								126.2	0.48
Sulfur dioxide	SO_2	77.7	430.7	122	0.246	197.7	4.50		
Ammonia	NH_3	111.5	405.6	72.5	0.250	195.4	3.48		
Argon	A	48.0	150.7	75.2	−0.002	83.8	1.69		
Methanol	CH_3OH	78.5	513.2	118.0	0.556	175.4	2.17		

Source: Ref. 3

Nomenclature

f	Fugacity of pure component	atm.
$k_{1,2}$	Binary parameter in gas phase	—
$\ell_{1,2}$	Solute/solvent interaction parameter	—
P	Pressure	atm.
P_r	Reduced pressure	—
R	Gas constant	1.987 cal/mole K
ΔS	Molar entropy change	cal/mole K
t	Temperature	°C
T	Temperature	K
T_r	Reduced temperature	—
V	Liquid molar volume	cm^3/mole
X	Mole fraction in liquid phase	—
δ	Solubility parameter	$(cal/cm^3)^{1/2}$
ϕ	Volume fraction	—
γ	Activity coefficient	—
ω	Pitzer's acentric factor	—

Superscripts

L	Liquid state
S	Solid state
n	Iteration number

Subscripts

1	Solvent
2	Solute
F	Fusion
M	Normal melting point
TR	Transition point
C	Critical

Program listing and comments **Table III**

Routine A: Handles data input for the solvent

Step	Key	Code
001	*LBLA	21 11
002	STO4	35 04
003	R↓	-31
004	STO2	35 02
005	R↓	-31
006	STO0	35 00
007	R↓	-31
008	STO1	35 01
009	R/S	51
010	STO5	35 05
011	R↓	-31
012	STO3	35 03
013	RTN	24

Routine B: Handles data input for the solute

Step	Key	Code
014	*LBLB	21 12
015	P⇄S	16-51
016	GSBA	23 11
017	P⇄S	16-51
018	RTN	24

Routine C: Stores $\ell_{1,2}$

Step	Key	Code
019	*LBLC	21 13
020	STOC	35 13
021	RTN	24

Routine D

Flag is set

Step	Key	Code
022	*LBLD	21 14
023	P⇄S	16-51
024	STO9	35 09
025	R↓	-31
026	STO6	35 06
027	SF1	16 21 01
028	P⇄S	16-51
029	RTN	24

Routine E: The main calculation. It derives the solubility by an iterative method and calls on subroutines b and e for calculation of δ and V.

Step	Key	Code
030	*LBLE	21 15
031	2	02
032	7	07
033	3	03
034	+	-55
035	STOD	35 14
036	P⇄S	16-51
037	CLX	-51
038	F1?	16 23 01
039	GSB3	23 03
040	1	01
041	RCL3	36 03
042	RCLD	36 14
043	÷	-24
044	-	-45
045	RCL5	36 05
046	x	-35
047	+	-55
048	STOB	35 12
049	GSBb	23 16 12
050	GSBe	23 16 15
051	P⇄S	16-51
052	GSBb	23 16 12
053	GSBe	23 16 15
054	P⇄S	16-51
055	RCL7	36 07
056	RCL7	36 07
057	P⇄S	16-51
058	RCL7	36 07
059	x	-35
060	RCLC	36 13
061	x	-35
062	2	02
063	x	-35
064	X⇄Y	-41
065	CHS	-22
066	RCL7	36 07
067	+	-55
068	X²	53
069	+	-55
070	RCLD	36 14
071	÷	-24
072	2	02
073	÷	-24
074	STOA	35 11
075	.	-62
076	1	01

Routine 1: Establishes the iterative loop in Routine E

Step	Key	Code
077	*LBL1	21 01
078	STOE	35 15
079	RCLE	36 15
080	1/X	52
081	1	01
082	-	-45
083	RCL8	36 08
084	x	-35
085	1/X	52
086	P⇄S	16-51
087	RCL8	36 08
088	1/X	52
089	+	-55
090	X²	53
091	RCL8	36 08
092	x	-35
093	1/X	52
094	P⇄S	16-51
095	RCLA	36 11
096	x	-35
097	CHS	-22
098	RCLB	36 12
099	+	-55
100	e^x	33
101	STOI	35 46
102	RCLE	36 15
103	÷	-24
104	1	01
105	-	-45
106	ABS	16 31
107	.	-62
108	0	00
109	1	01
110	X>Y?	16-34
111	GTO2	22 02
112	RCLI	36 46
113	GTO1	22 01

Subroutine 3: Takes account of the transition effect if $T < T_{tr}$

Step	Key	Code
114	*LBL3	21 03
115	1	01
116	RCL6	36 06
117	RCLD	36 14
118	÷	-24
119	-	-45
120	0	00
121	X≤Y?	16-35
122	RTN	24
123	X⇄Y	-41
124	RCL9	36 09
125	x	-35
126	RTN	24

Routine 2: Displays solubility X_2

Step	Key	Code
127	*LBL2	21 02
128	RCLI	36 46
129	RTN	24

Subroutine b: Completes the calculation of δ for solvent and solute

Step	Key	Code
130	*LBLb	21 16 12
131	RCL4	36 04
132	3	03
133	.	-62
134	3	03
135	3	03
136	9	09
137	x	-35
138	2	02
139	.	-62
140	0	00
141	4	04
142	-	-45
143	RCL4	36 04
144	x	-35
145	.	-62
146	6	06
147	3	03
148	1	01
149	2	02
150	-	-45
151	RCLD	36 14
152	RCL0	36 00
153	÷	-24
154	X²	53
155	x	-35
156	1	01
157	.	-62
158	8	08
159	2	02
160	RCL4	36 04
161	1	01
162	.	-62
163	3	03
164	4	04
165	5	05
166	x	-35
167	-	-45
168	RCL4	36 04
169	x	-35
170	+	-55
171	1	01
172	.	-62
173	2	02
174	1	01
175	6	06
176	5	05
177	+	-55
178	RCL1	36 01
179	√X	54
180	x	-35
181	STO7	35 07
182	RTN	24

Subroutine e: Provides the calculation of V for solvent and solute

Step	Key	Code
183	*LBLe	21 16 15
184	RCL4	36 04
185	.	-62
186	1	01
187	6	06
188	9	09
189	x	-35
190	CHS	-22
191	.	-62
192	1	01
193	9	09
194	6	06
195	+	-55
196	RCL4	36 04
197	x	-35
198	.	-62
199	1	01
200	4	04
201	5	05
202	2	02
203	RCLD	36 14
204	RCL0	36 00
205	÷	-24
206	X²	53
207	x	-35
208	.	-62
209	3	03
210	3	03
211	9	09
212	+	-55
213	RCL4	36 04
214	.	-62
215	1	01
216	5	05
217	x	-35
218	-	-45
219	RCL2	36 02
220	x	-35
221	STO8	35 08
222	RTN	24
223	R/S	51

(Continued from p. 199)

the deviation from the assumed geometric mean of the critical temperature, such that:

$$T_{C1,2} = (T_{C1} \cdot T_{C2})^{1/2}(1 - k_{1,2}) \qquad (6)$$

The two binary parameters $k_{1,2}$ and $\ell_{1,2}$ do not reflect the same kind of interactions, but for molecules of similar size we can use $\ell_{1,2} = k_{1,2}$ as an approximation.

3. If no specific information is available at all, take $\ell_{1,2} = 0.05$ and increase this value with differences in molecular size and chemical structure. Likewise, decrease it if there are specific interactions (such as hydrogen bonds) between molecules of solute and solvent (see Examples 1 and 2).

The program

The program listing shown in Table III should be keyed into the calculator and stored on a magnetic card.

Storage registers — **Table V**

Storage register	Value	Storage register	Value
P0	T_{C1}	S0	T_{C2}
P1	P_{C1}	S1	P_{C2}
P2	V_{C1}	S2	V_{C2}
P3	T_{F1}	S3	T_{F2}
P4	ω_1	S4	ω_2
P5	$\Delta S_{F2}/R$	S5	$\Delta S_{F2}/R$
P6	Not used	S6	T_{TR}
P7	δ_1	S7	δ_2
P8	V_1	S8	V_2
P9	Not used	S9	$\Delta S_{TR}/R$
A	Intermediate value	D	T
B	Intermediate value	E	$X_2{}^n$
C	$\ell_{1,2}$	I	$X_2{}^{n+1}$

User's instructions for general case — **Table IV**

Step	Value	Unit	Key
Store data for solvent	Critical pressure	atm	P_{C1} ↑
	Critical temperature	K	T_{C1} ↑
	Critical volume	cm^3/mole	V_{C1} ↑
	Acentric factor	–	ω_1 A
	Melting point	K	T_{F1} ↑
	Molar entropy of fusion	–	$\Delta S_{F1}/R$ R/S
Store data for source	Critical pressure	atm	P_{C2} ↑
	Critical temperature	K	T_{C2} ↑
	Critical volume	cm^3/mole	V_{C2} ↑
	Acentric factor	–	ω_2 B
	Melting point	K	T_{F2} ↑
	Molar entropy of fusion	–	$\Delta S_{F2}/R$ R/S
Store $\ell_{1,2}$	Interaction parameter	–	$\ell_{1,2}$ C
Solid-phase transition	Transition temperature	K	T_{TR} ↑
	Molar entropy of transition	–	$\Delta S_{TR}/R$ D
Begin computation	Temperature	°C	E → X_2 Display

Solubilities of solid hydrocarbons in liquid nitrogen — **Table VI**

	Solvent: Nitrogen	Solute: Methane	Ethane	Propane	Isobutane	Ethylene	Propylene	Butene	Acetylene
P_C	33.5 ↑	45.8 ↑	48.3 ↑	42.0 ↑	36.0 ↑	50.5 ↑	45.4 ↑	38.7 ↑	61.7 ↑
T_C	126.2 ↑	191.1 ↑	305.6 ↑	370.0 ↑	408.1 ↑	283.1 ↑	365.1 ↑	419.5 ↑	308.7 ↑
V_C	90 ↑	99 ↑	148 ↑	200 ↑	263 ↑	124 ↑	181 ↑	241 ↑	113 ↑
ω	0.04 A	0.013 B	0.105 B	0.152 B	0.192 B	0.087 B	0.143 B	0.203 B	0.186 B
T_F	63.2 ↑	90.7 ↑	89.9 ↑	85.5 ↑	113.7 ↑	104.0 ↑	87.9 ↑	87.8 ↑	192.4 ↑
ΔS_F	1.37 R/S	1.25 R/S	3.82 R/S	4.96 R/S	4.80 R/S	3.88 R/S	4.11 R/S	5.27 R/S	2.55 R/S
$\ell_{1,2}$		0.05 C	0.05 C	0.05 C	0.05 C	0.05 C	0.05 C	0.05 C	0.05 C
t		−196 E	−196 E	−196 E	−196 E	−196 E	−196 E	−196 E	−196 E
X_2 (Display)		0.627	2.34×10^{-3}	6.09×10^{-4}	4.95×10^{-5}	2.79×10^{-3}	4.98×10^{-4}	1.08×10^{-4}	3.83×10^{-6}
X_2 (Experimental)*		0.63	7.76×10^{-3}	1.0×10^{-3}	1.0×10^{-4}	2.02×10^{-3}	7.73×10^{-4}	1.0×10^{-4}	4.6×10^{-6}

*Source: Ref. 4

Solubility of solid hydrogen sulfide in liquid methane — **Table VII**

	Step 1 Solvent: CH_4	Step 2 Source: H_2O	Step 3 Interaction	Step 4 Transition	Step 5 Computation
P_C	45.8 ↑	88.9 ↑	$\ell_{1,2}$ 0.06 C	T_{TR} 126.2 ↑	t = −154°C E
T_C	191.1 ↑	373.6 ↑		$\Delta S_{TR}/R$ 0.48 D	
V_C	99 ↑	97.7 ↑			X_2 (Display) = 0.00128
ω	0.013 A	0.100 B			X_2 (Exp.) = 0.0012*
T_F	90.7 ↑	187.6 ↑			
$\Delta S_F/R$	1.25 R/S	1.52 R/S			

(Clear Flag 1 by h CF 1 after each solute example)

*Source: Ref. 5.

Solubility of solid benzene in propane — **Table VIII**

	Step 1 Solvent: Propane	Step 2 Solute: Benzene
P_C	42 ↑	48.6 ↑
T_C	370 ↑	562.6 ↑
V_C	200 ↑	260 ↑
ω	0.152 A	0.215 B
T_F	85.5 ↑	278.15 ↑
$\Delta S_F/R$	4.96 R/S	4.25 R/S

Step 3

Try $\ell_{1,2}$ to fit experimental data at −75.3°C

$\ell_{1,2}$ = 0.05 C	t = −75.3°C E	→ X_2 = 0.00139	Low
$\ell_{1,2}$ = 0.01 C	t = −75.3°C E	→ X_2 = 0.05798	High
$\ell_{1,2}$ = 0.02 C	t = −75.3°C E	→ X_2 = 0.04074	O.K.

Step 4

Compute X_2

t = −142.5°C E → X_2 (Display) = 0.00111

X_2 (Exper.)* = 0.00113

*Source: Ref. 6.

Key **A** is used for storage of physical data for the pure solvent. Key **B** is used the same way for the pure solute. Key **C** is used for the solute-solvent interaction factor (if available) or 0.05 as standard. Key **D** may be used for a solid-phase transition in the solute structure.

After the temperature has been entered, Key **E** will produce molar solubility as output.

Table IV summarizes the user's instructions. Table V shows the registers after running the program.

Examples

1. **Estimating solubility (without transition of phase)**—Let us determine the orders of magnitude of the solubilities of solidified methane, ethane, propane, isobutane, ethylene, propylene, butene and acetylene in liquid nitrogen at 77 K (−196°C).

Before running the program, it is necessary to select from Table II the values P_C, T_C, V_C, ω, T_F, $\Delta S_{F/R}$ for solute and solvent.

The results are shown in Table VI and, in the absence of specific data, a value of 0.05 is used for $\ell_{1,2}$.

2. **Estimating solubility with transition of phase**—Estimate the solubility of solid hydrogen sulfide in liquid methane at −154°C.

From Table II, it appears that H_2S undergoes a solid-phase transition at $t = -147$°C.

Due to the chemical difference in solvent and solute, we can assume a higher value for $\ell_{1,2}$, for example, $\ell_{1,2} = 0.06$.

Results are shown in Table VII.

3. **Correlating data with one known point**—What is the solubility of solid benzene in propane at −142.5°C if the solubility is $X_2 = 0.0398$ at −75.3°C?

First, we determine by trial and error the $\ell_{1,2}$ that gives the best fit with the experimental point. This iterative procedure is easily done, using the program. We find that $\ell_{1,2} = 0.02$.

Results are shown in Table VIII.

Comment*

Sir: The article, "Program aids cryogenic solubility calculations," in your July 13, 1981 issue (pp. 127–131), has a step "+" (Code -55) missing between Steps 202 and 203. This invalidates the coding for V/Vc (Table I, p. 127) and changes the answers for all except the text example, "... X_2 = 0.0398 at -75.3°C?", on p. 131. While the examples give approximate answers, the published program does not reflect the published formulation.

ELMER B. CLAUSEN
Buffalo, N.Y.

Author replies

There is a discrepancy between the formulation and the listing. For optimal computation, the final expression selected for V/Vc (Table I) was

$$V/V_c = 0.1452T_r^2 + 0.339 - 0.15\omega$$

Accordingly, Lines 184 to 197 in Label e may be deleted (in fact, they are not used when LBL e is executed).

The text and the examples are unchanged.

PATRICE LABRUN
Paris, France

*Letter originally published January 11, 1982.

For TI-58/59 users

The TI-58/59 version of the program appears in Table IX. Storage registers for the TI version are found in Table X, and user instructions are in Table XI. The program is run in a similar manner to the HP-67/97 version, but with some variation in the use of the keys.

The same order of entering data is followed for the TI-58/59 version as for the HP-67/97 program. Therefore, the examples will not be repeated. However, to show the outputs for the TI-58/59 version, Table XII shows some of the results (the TI-58/59 yields many more significant figures than are shown in Tables VI-VII). Outputs are given for methane and ethane in Example 1 (in Table VI), and for Example 2 (in Table VII) and Example 3 (Table VIII).

Program listing for TI version **Table IX**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	054	91	R/S	108	42	STO	162	42	STO	216	18	18
001	11	A	055	76	LBL	109	11	11	163	08	08	217	35	1/X
002	42	STO	056	15	E	110	43	RCL	164	53	(	218	54	)
003	01	01	057	85	+	111	12	12	165	43	RCL	219	33	X²
004	91	R/S	058	02	2	112	48	EXC	166	07	07	220	65	×
005	42	STO	059	07	7	113	02	02	167	65	×	221	43	RCL
006	00	00	060	03	3	114	42	STO	168	43	RCL	222	18	18
007	91	R/S	061	95	=	115	12	12	169	17	17	223	54	)
008	42	STO	062	42	STO	116	43	RCL	170	65	×	224	35	1/X
009	02	02	063	24	24	117	07	07	171	43	RCL	225	65	×
010	91	R/S	064	25	CLR	118	48	EXC	172	23	23	226	43	RCL
011	42	STO	065	87	IFF	119	17	17	173	65	×	227	21	21
012	04	04	066	01	01	120	43	RCL	174	02	2	228	94	+/-
013	91	R/S	067	24	CE	121	08	08	175	85	+	229	85	+
014	42	STO	068	76	LBL	122	48	EXC	176	53	(	230	43	RCL
015	03	03	069	44	SUM	123	18	18	177	43	RCL	231	22	22
016	91	R/S	070	85	+	124	71	SBR	178	07	07	232	54	)
017	42	STO	071	53	(	125	34	√X	179	75	-	233	22	INV
018	05	05	072	01	1	126	71	SBR	180	43	RCL	234	23	LNX
019	91	R/S	073	75	-	127	33	X²	181	17	17	235	42	STO
020	76	LBL	074	53	(	128	43	RCL	182	54	)	236	26	26
021	12	B	075	43	RCL	129	04	04	183	33	X²	237	55	÷
022	42	STO	076	13	13	130	48	EXC	184	54	)	238	43	RCL
023	11	11	077	55	÷	131	14	14	185	55	÷	239	25	25
024	91	R/S	078	43	RCL	132	42	STO	186	43	RCL	240	75	-
025	42	STO	079	24	24	133	04	04	187	24	24	241	01	1
026	10	10	080	54	)	134	43	RCL	188	55	÷	242	95	=
027	91	R/S	081	54	)	135	00	00	189	02	2	243	50	I×I
028	42	STO	082	65	×	136	48	EXC	190	54	)	244	32	X:T
029	12	12	083	43	RCL	137	10	10	191	42	STO	245	93	.
030	91	R/S	084	15	15	138	42	STO	192	21	21	246	00	0
031	42	STO	085	95	=	139	00	00	193	93	.	247	01	1
032	14	14	086	42	STO	140	43	RCL	194	01	1	248	32	X:T
033	91	R/S	087	22	22	141	01	01	195	76	LBL	249	22	INV
034	42	STO	088	71	SBR	142	48	EXC	196	35	1/X	250	77	GE
035	13	13	089	34	√X	143	11	11	197	42	STO	251	42	STO
036	91	R/S	090	71	SBR	144	42	STO	198	25	25	252	43	RCL
037	42	STO	091	33	X²	145	01	01	199	53	(	253	26	26
038	15	15	092	43	RCL	146	43	RCL	200	53	(	254	61	GTO
039	91	R/S	093	14	14	147	02	02	201	53	(	255	35	1/X
040	76	LBL	094	48	EXC	148	48	EXC	202	53	(	256	76	LBL
041	13	C	095	04	04	149	12	12	203	43	RCL	257	24	CE
042	42	STO	096	42	STO	150	42	STO	204	25	25	258	01	1
043	23	23	097	14	14	151	02	02	205	35	1/X	259	75	-
044	91	R/S	098	43	RCL	152	43	RCL	206	75	-	260	43	RCL
045	76	LBL	099	10	10	153	07	07	207	01	1	261	16	16
046	14	D	100	48	EXC	154	48	EXC	208	54	)	262	55	÷
047	42	STO	101	00	00	155	17	17	209	65	×	263	43	RCL
048	16	16	102	42	STO	156	42	STO	210	43	RCL	264	24	24
049	91	R/S	103	10	10	157	07	07	211	08	08	265	95	=
050	42	STO	104	43	RCL	158	43	RCL	212	95	=	266	32	X:T
051	19	19	105	11	11	159	08	08	213	35	1/X	267	00	0
052	86	STF	106	48	EXC	160	48	EXC	214	85	+	268	22	INV
053	01	01	107	01	01	161	18	18	215	43	RCL	269	77	GE

(Continued) Table IX

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
270	44	SUM	297	65	×	324	43	RCL	351	93	.	378	24	24
271	32	X⇌T	298	03	3	325	00	00	352	02	2	379	55	÷
272	65	×	299	93	.	326	54	)	353	01	1	380	43	RCL
273	43	RCL	300	03	3	327	33	X²	354	06	6	381	00	00
274	19	19	301	03	3	328	95	=	355	05	5	382	54	)
275	95	=	302	09	9	329	85	+	356	54	)	383	33	X²
276	61	GTO	303	75	−	330	53	(	357	65	×	384	85	+
277	44	SUM	304	02	2	331	01	1	358	43	RCL	385	93	.
278	76	LBL	305	93	.	332	93	.	359	01	01	386	03	3
279	42	STO	306	00	0	333	08	8	360	34	√X	387	03	3
280	43	RCL	307	04	4	334	02	2	361	95	=	388	09	9
281	26	26	308	54	)	335	75	−	362	42	STO	389	75	−
282	22	INV	309	65	×	336	43	RCL	363	07	07	390	43	RCL
283	86	STF	310	43	RCL	337	04	04	364	92	RTN	391	04	04
284	01	01	311	04	04	338	65	×	365	76	LBL	392	65	×
285	99	PRT	312	75	−	339	01	1	366	33	X²	393	93	.
286	98	ADV	313	93	.	340	93	.	367	53	(	394	01	1
287	91	R/S	314	06	6	341	03	3	368	53	(	395	05	5
288	76	LBL	315	03	3	342	04	4	369	93	.	396	54	)
289	34	√X	316	01	1	343	05	5	370	01	1	397	65	×
290	53	(	317	02	2	344	54	)	371	04	4	398	43	RCL
291	53	(	318	54	)	345	65	×	372	05	5	399	02	02
292	53	(	319	65	×	346	43	RCL	373	02	2	400	95	=
293	53	(	320	53	(	347	04	04	374	54	)	401	42	STO
294	53	(	321	43	RCL	348	54	)	375	65	×	402	08	08
295	43	RCL	322	24	24	349	85	+	376	53	(	403	92	RTN
296	04	04	323	55	÷	350	01	1	377	43	RCL			

Data storage locations:	Solvent		Solute
Critical pressure	01		11
Critical temperature	00		10
Critical volume	02		12
Acentric factor	04		14
Fusion temperature	03		13
Molal entropy change	05		15
Interaction		23	
Transition temperature		16	
Transition entropy		19	
Temperature		24	

User instructions for the TI version **Table X**

Step	Value	Unit	Key
Enter program			
Store data for solvent	Critical pressure	atm	**A**
	Critical temperature	K	**R/S**
	Critical volume	cm^3/mole	**R/S**
	Acentric factor	—	**R/S**
	Melting point	K	**R/S**
	Molar entropy change	—	**R/S**
Store data for solute	Critical pressure	atm	**B**
	Critical temperature	K	**R/S**
	Critical volume	cm^3/mole	**R/S**
	Acentric factor	—	**R/S**
	Melting point	K	**R/S**
	Molar entropy change	—	**R/S**
Store l_{12}	Interaction parameter	—	**C**
Solid-phase transition	If so, store:		
	Transition temperature	K	**D**
	Molar entropy of transition	—	**R/S**
Begin computation	Temperature	°C	**E**

Note: Data for solvent and solute are retained by the program, and solubilities at other temperatures or interactions may be made by entering only the data that need to be changed.

Storage registers for TI version **Table XI**

Storage Register	Value	Storage Register	Value
01	T_{C1}	11	T_{C2}
00	P_{C1}	10	P_{C2}
02	V_{C1}	12	V_{C2}
03	T_{F1}	13	T_{F2}
04	ω_1	14	ω_2
05	$\Delta S_{F1}/R$	15	$\Delta S_{F2}/R$
23	l_{12}	16	T_{TR}
19	$\Delta S_{TR}/R$	24	t

Examples for TI version **Table XII**

Example 1 **Solute**	x_2
Methane	.6265615084
Ethane	.0023427487
Example 2	
$x_2 =$	.0012806334
Example 3	
l_{12}	x_2
0.05	.0139246261
0.01	.0579814921
0.02	.0407416724
$t = -142.5°C$, $x_2 =$	0.001105652

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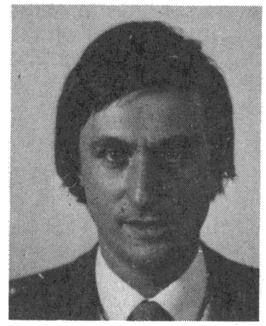
The author



Patrice Lebrun was formerly a process engineer with L'Air Liquide. His work involved the application of cryogenics to gas purification, liquefaction of natural gas, and refrigerated absorbers. Previously, he was a process engineer with Litwin (France), where he was involved in bulk polymerization of polystyrene. He received a B.S. degree in organic chemistry from the University of Lyon and an M.S. in chemical engineering from Toulouse University.

Program calculates hydrocyclone efficiency

This HP-41C program determines the circulating load, efficiency of separation for defined size fractions, and the sharpness of separation.

Frank H. Merrill, *Aguirre Engineers, Inc.*

☐ The hydrocyclone, a widely used classification device for performing size separations on mineral and chemical slurries, operates on a centrifugal principal. The slurry is fed under pressure through a tangential inlet in the cylindrical section (see Fig. 1), setting up a rotational motion, and forming a primary vortex along the inside surface wall that is aimed at the apex of the conical section. Inside this primary vortex, an upward-moving secondary vortex forms in line with the vortex finder. This secondary vortex carries most of the liquid out the overflow.

As the slurry is fed to the hydrocyclone, the induced rotation sets up a centrifugal force that causes the coarse particles to settle against the wall and be carried toward the apex for discharge in the underflow. The less-coarse particles pass into the secondary vortex near the apex. In the secondary vortex, higher circumferential velocities cause a substantial increase in the centrifugal force to which the solids are subjected. This results in another settling out of particles, which pass back into the primary vortex for discharge. The residual fine material moves up the secondary vortex and passes out of the hydrocyclone through the overflow outlet [*1*].

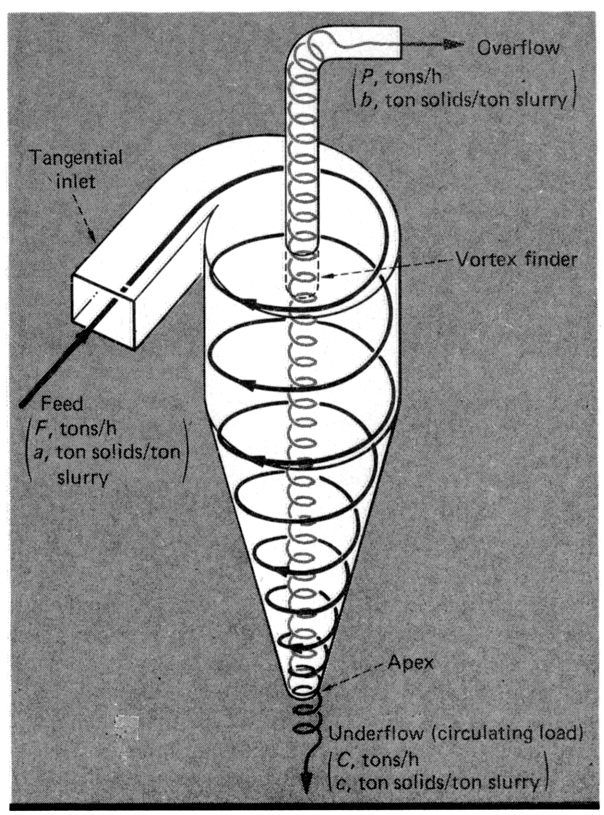
One of the great advantages of the hydrocyclone is that the composition of the two products, the overflow and the underflow, can be varied with relative ease. Depending on the requirements of the system, a hydrocyclone can be operated to produce either a coarse/fine separation or a solid/liquid separation [*3*].

Mineral processing applications

The most common use of the hydrocyclone in mineral processing is to control the size of the final product from a grinding circuit. All mineral separations require liberation of the valuable mineral from the gangue, or worthless material in the ore. Depending on the specific ore, complete liberation may be accomplished at 35 mesh (425 μm), or it may require grinding to as fine as 400 mesh (37 μm).

For all but the very coarsest of grinds, the usual method is to use ball or rod mills. The most common configuration is a single mill closed by a hydrocyclone system (see Fig. 2). In this system, the coarse ore is fed to the mill, and the mill discharge is pumped through the hydrocyclone. The hydrocyclone is set to operate so that material fine enough to be completely liberated passes out through the overflow and on to further processing. The oversize material exits through the underflow and is returned to the mill for further grinding.

Another frequently encountered configuration is an open rod mill followed by a closed ball mill system (see Fig. 3). In this system, coarse ore is fed to the rod mill for a first stage of grinding, the discharge from which is then pumped to the hydrocyclone for sizing. The overflow from the hydrocyclone passes on to further processing, while the underflow is sent to the ball mill for fur-



Hydrocyclone construction and flow pattern Fig. 1

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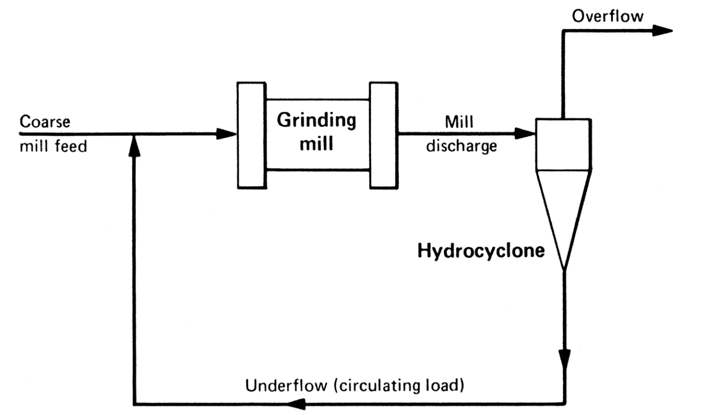
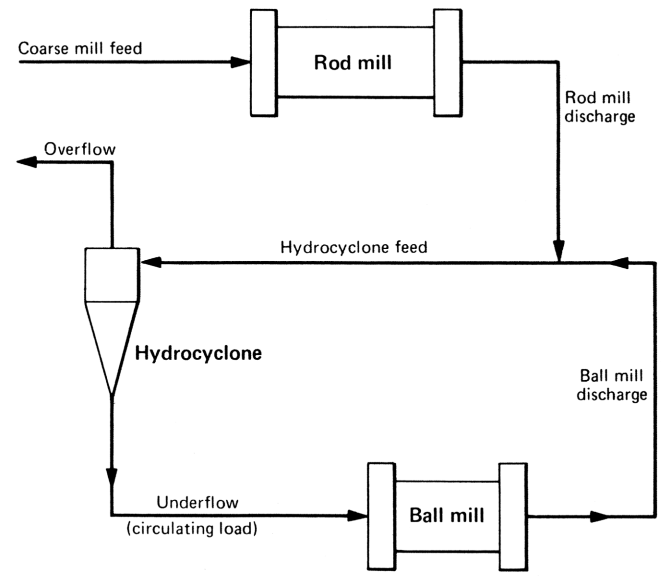
Nomenclature

a Solids content of hydrocyclone feed, tons solids/ton slurry
b Solids content of hydrocyclone overflow, tons solids/ton slurry
C Hydrocyclone underflow (circulating load), tons solids/h
c Solids content in hydrocyclone underflow, tons solids/ton slurry
d Particle size, microns
d_s Screen aperture size, microns.
d_T Particle size for which Tromp values are calculated, microns.
d_{25} Particle size for which hydrocyclone efficiency equals 25%, microns.
d_{50} Particle size for which hydrocyclone efficiency equals 50%, microns.
d_{75} Particle size for which hydrocyclone efficiency equals 75%, microns.
E Hydrocyclone efficiency for a given particle size, percent
F Hydrocyclone feed, tons solids/h
I Imperfection (sharpness of cut).
P Hydrocyclone overflow, tons solids/h
R_b Weight fraction of overflow solids retained by any given screen, from screen analysis of hydrocyclone overflow, grams retained/gram composite screen sample
R_c Weight fraction of underflow solids retained by any given screen, from screen analysis of hydrocyclone underflow, grams retained/gram composite screen sample
T Differential mass recovery for a given size fraction (Tromp value)
W Weight of solids retained by any given screen, grams
γ Specific gravity of solid material
θ Overall mass recovery

Subscripts
i Component i



Simple closed mill system **Fig. 2**



Open rod mill followed by closed ball mill grinding system **Fig. 3**

ther grinding. The ball mill discharge then joins the rod mill discharge and is pumped to the hydrocyclone.

A less frequently encountered use of hydrocyclones in the mineral processing industry is the actual concentration of the valuable mineral. This application is seen most frequently in the nonmetallic minerals industry and is especially prevalent in the preparation of kaolin and other clay materials [*1*].

In the closed-circuit grinding of ores, a universally encountered operating parameter is the *circulating load.* The circulating load, defined as the material returned to the grinding mill from the classifier, is expressed as a percentage of the coarse ore feed [*2*]. In general, mill operators try to keep the circulating load in the range of 150%–300%, though exceptions are common [*4*].

Increasing the circulating load has the effects of lowering the sharpness of the classifier separation, and producing a coarser grind in the mill [*4*]. As the circulating load continues to increase, the mill finally overloads. When this occurs, coarse feed to the mill must be cut off until the mill can grind through the overload. Conversely, if the circulating load decreases, a finer grind and sharper classifier separation will result, but the coarse feedrate will be lowered. Thus the regulation of the circulating load becomes a matter of balancing the requirements for mill throughput, fineness of grind, and sharpness of separation.

Hydrocyclone efficiency

Hydrocyclone efficiency is almost universally defined in terms of the underflow for each size fraction. Thus a hydrocyclone will have a series of efficiency values ranging from close to 1.0 at coarse sizes to approaching 0.0 at very fine sizes.

The *split point* (d_{50}) for a hydrocyclone is the particle size at which 50% of the material is overflow, and 50% is underflow. This point depends on hydrocyclone dimensions, solids content of the feed slurry, and feed pressure [1,6]. The hydrocyclone efficiency at the split point is by definition 50%. Two other sizes, d_{75} and d_{25}, are the particle sizes at which 75% and 25%, respectively, report to the underflow.

Any consideration of hydrocyclone operation must begin with a mass balance. If a simple closed-circuit system is considered, with the solids contents of the three streams and the coarse ore feedrate known, it is possible to determine the hydrocyclone feedrate and the circulating load. This is done by evaluating the solids mass balance and the overall mass balance.

It must first be remembered that the grinding mill-hydrocyclone system will be operating in a steady-state condition. Thus, if the coarse ore feedrate is known, the hydrocyclone overflow is also known.

The solids mass balance relates the tons of solids/h in the three streams:

$$F = P + C \tag{1}$$

Note that the underflow is the circulating load for this system.

The overall mass balance relates the tons of slurry/h:

$$\frac{F}{a} = \frac{P}{b} + \frac{C}{c} \tag{2}$$

By solving Eq. (1) and (2) simultaneously, the two unknown solids flowrates can be determined.

Determining the efficiencies is a multistep process. The first step is to determine the overall mass recovery for the hydrocyclone. The mass recovery can be determined from the solids contents of the three streams, and the specific gravity of the solids [1]:

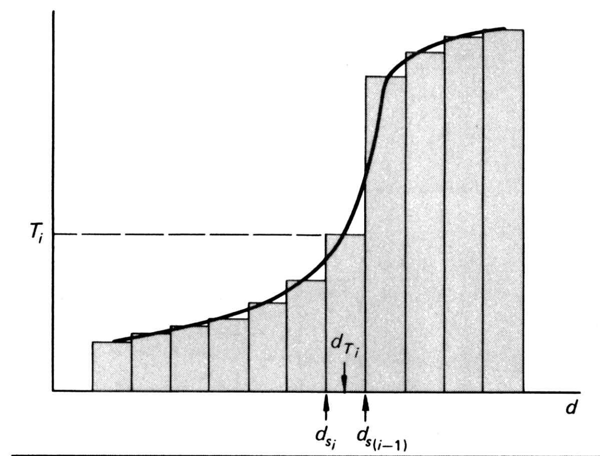
$$\theta = \left(\frac{a-b}{c-b}\right)\cdot\left(\frac{\gamma-c}{\gamma-a}\right) \tag{3}$$

This gives the fraction of the total solids in the feed that report to the underflow. Once the overall mass recovery has been determined, if screen analyses of the overflow and underflow solids are available, it is possible to calculate the differential mass recovery or *Tromp value*. The Tromp value is the mass recovery for a given size fraction of the solid material in the feed, and is calculated thus [1]:

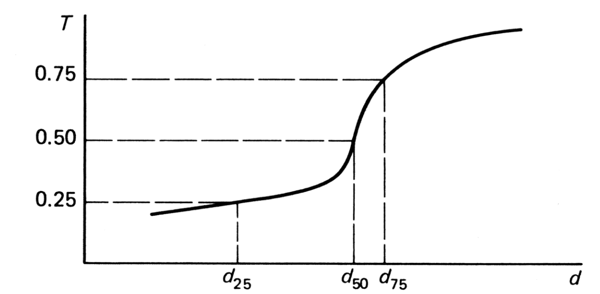
$$T_i = \frac{\theta R_{c_i}}{[\theta R_{c_i}] + [(1-\theta)\cdot R_{b_i}]} \tag{4}$$

The *Tromp curve* is a semilogarithmic plot of the Tromp values (T_i) versus the median particle size for each size fraction (see Fig. 4). From the Tromp curve, the split point (d_{50}) can be determined by locating the particle size for which $T_i = 0.50$. If the screen data are satisfactory, it is also possible to determine d_{25} and d_{75} from the curve (see Fig. 5).

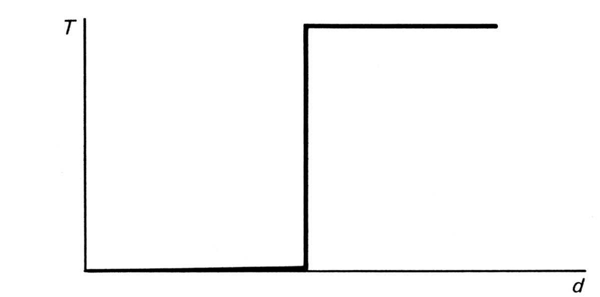
The Tromp curve presents a visual indication of how effectively the hydrocyclone is doing its job. Ideally, the curve would show a vertical drop at the desired separation size, as shown in Fig. 6. A curve showing a nearly horizontal line would indicate that the hydrocyclone is doing almost nothing in the way of size classification (see Fig. 7) [2]. If only general results or trends are re-



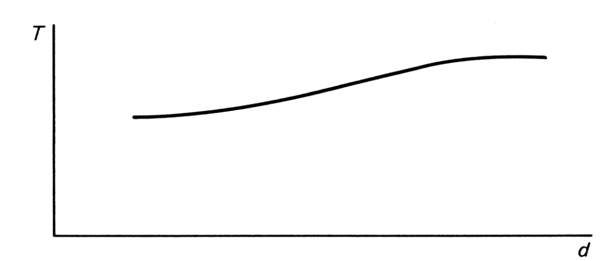
Construction of the Tromp curve **Fig. 4**



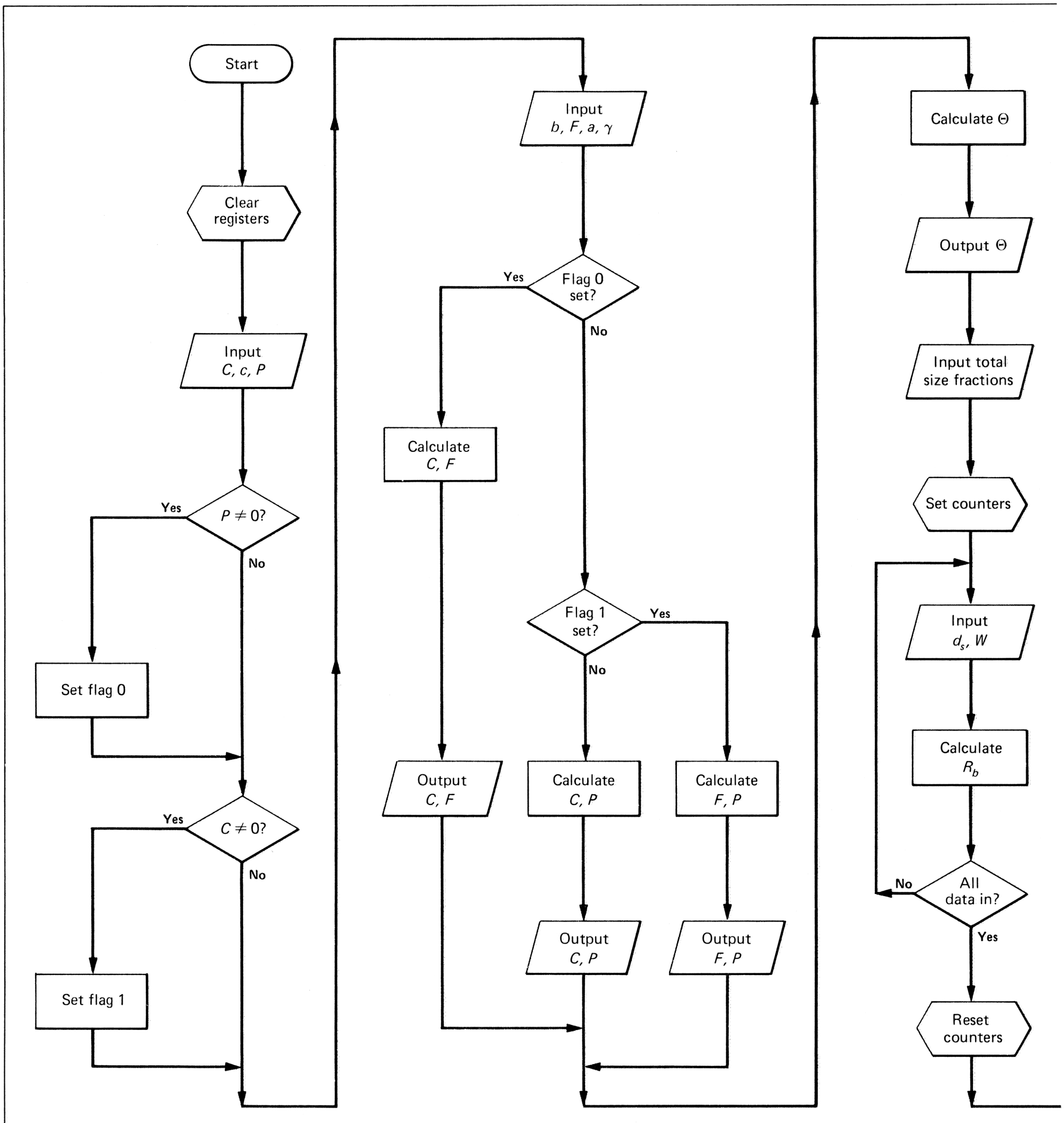
Using the Tromp curve to determine the values of d_{25}, d_{50}, and d_{75} **Fig. 5**



Tromp curve for perfect hydrocyclone operation **Fig. 6**



Tromp curve indicating exceedingly poor hydrocyclone operation **Fig. 7**



Flowchart for hydrocyclone calculations

quired, the Tromp curve can serve as a fully satisfactory indicator of hydrocyclone efficiency.

The equation put forth by G. I. Bennett, shown below, provides excellent results for the conditions of operation likely to be encountered in a mineral processing operation [6,7]:

$$E = 100[1.0 - \exp(-[(d/d_{50} - 0.115]^3)] \quad (5)$$

One immediate advantage of Bennett's equation over the Tromp curve is that only one piece of information from the Tromp curve is required: the value of d_{50}. This advantage is multiplied when it is remembered that the d_{50} value comes from the steepest, and most accurate, section of the Tromp curve. With Bennett's equation, once d_{50} is known, the hydrocyclone efficiency at any other size can be found with no difficulty. Additionally,

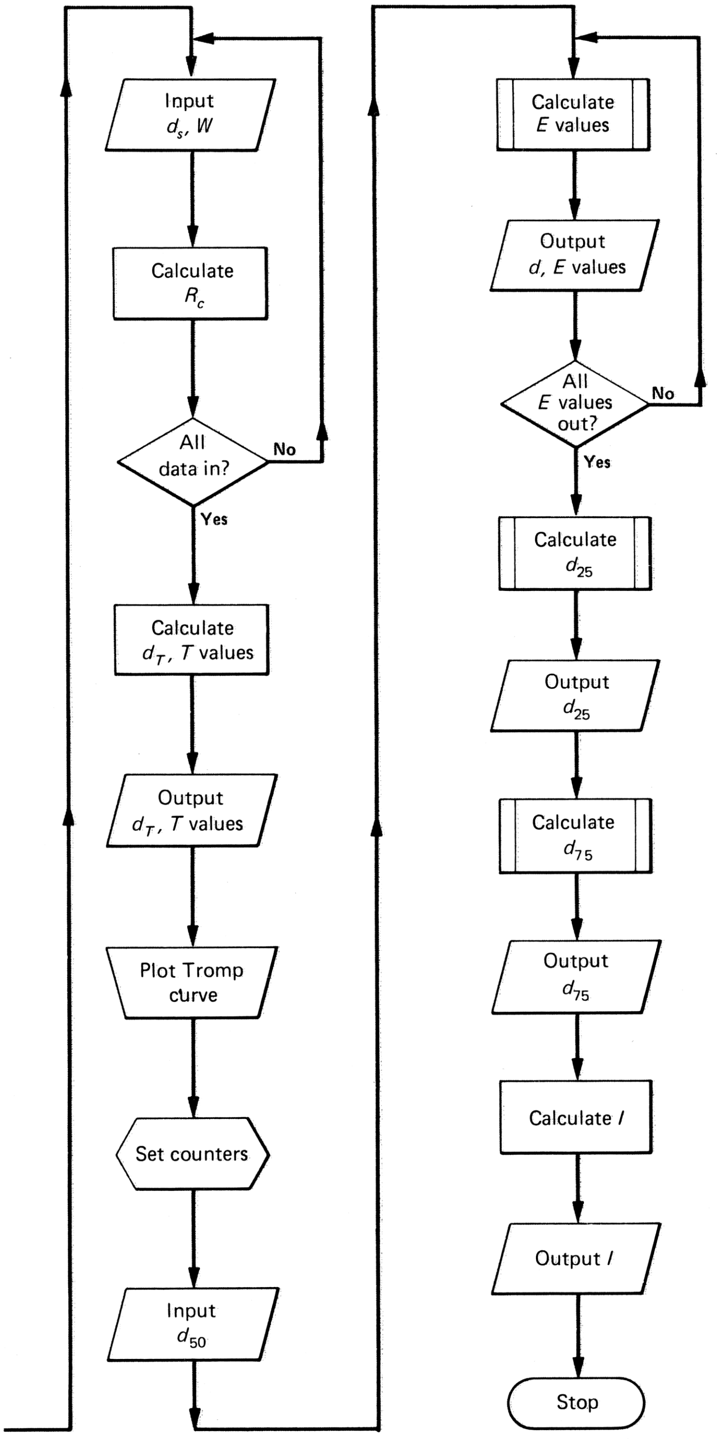
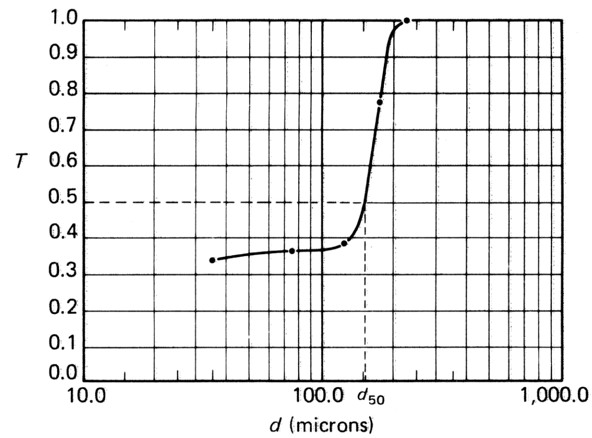


Fig. 8



Tromp curve generated with data from sample problem **Fig. 9**

in situations where an accurate value of d_{25} or d_{75} is required, the equation can readily be solved for particle size, d:

$$d = (\sqrt[3]{-\ln[1-(E/100)]} + 0.115)d_{50} \tag{6}$$

A final indicator of hydrocyclone performance is the sharpness of separation or the *imperfection, I*. The imperfection is a measure of how accurately sized the hydrocyclone products will be. The imperfection depends on d_{75}, d_{50}, and d_{25} [*1*]:

$$I = \frac{d_{75} - d_{25}}{2d_{50}} \tag{7}$$

From Eq. (7) and Fig. (6), it can be seen that if a hydrocyclone were to operate under ideal conditions, the value of I would be zero. In general, the steeper the Tromp curve, the lower the value of I. And the lower the imperfection, the more accurately sized the overflow and underflow solids will be.

The calculator program

The program is designed to run on the HP-41C or the HP-41CV calculator. If the HP-41C is used, either two HP-82106A Memory Modules or one HP-82170A Quad Memory are necessary. The HP-82104A Magnetic Card Reader, while not essential to program execution, will greatly speed up the process of entering the program.

Information required by the program includes the specific gravity of the solid material; the solids contents of the feed, overflow and underflow; the tons/h for one of the three streams; the number of size fractions; and the screen analyses for overflow and underflow. These analyses must include the size of the screens (in microns), and the weight in grams of each size fraction.

Using the data on solids flow and specific gravity, the program first calculates the tons/h for the other two streams, using Eq. (1) and (2). The overall mass recovery is then calculated via Eq. (3). The information from the screen analysis is entered at this point. The next step is the calculation of the Tromp values for each size fraction, using Eq. (4).

The calculator then outputs the mean size for each size fraction, followed by the Tromp value for that size fraction. This information should be copied down as it is presented. Upon completion of this series of outputs, the calculator will signal PLOT CURVE. At this point, it is necessary to plot the Tromp Curve and determine the

(Text continues on p. 214)

Calculator program for hydrocyclone circulating load, efficiencies, and sharpness of separation

```
01♦LBL "CYCLONE"
02♦LBL A
03 CLRG
04 FIX 1
05 "ENTER C, c, P"
06 PROMPT
07 STO 05
08 X≠0?
09 SF 00
10 RDN
11 STO 00
12 RDN
13 STO 03
14 X≠0?
15 SF 01
16 "ENTER b, F, a"
17 PROMPT
18 STO 01
19 RDN
20 STO 04
21 RDN
22 STO 02
23 "ENTER GAMMA"
24 PROMPT
25 STO 06
26 FS?C 00
27 GTO 01
28 FS?C 01
29 GTO 02
30 RCL 01
31 1/X
32 RCL 00
33 1/X
34 -
35 RCL 02
36 1/X
37 RCL 00
38 1/X
39 -
40 /
41 RCL 04
42 *
43 STO 05
44 CHS
45 RCL 04
46 +
47 STO 03
48 CLA
49 "C="
50 ARCL 03
51 AVIEW
52 PSE
53 PSE
54 PSE
55 CLA
56 "P="
57 ARCL 05
58 AVIEW
59 PSE
60 PSE
61 PSE
62 GTO 03
63♦LBL 01
64 RCL 02
65 1/X
66 RCL 00
67 1/X
68 -
69 RCL 01
70 1/X
71 RCL 00
72 1/X
73 -
74 /
75 RCL 05
76 *
77 STO 04
78 RCL 05
79 -
80 STO 03
81 CLA
82 "C="
83 ARCL 03
84 AVIEW
85 PSE
86 PSE
87 PSE
88 CLA
89 "F="
90 ARCL 04
91 AVIEW
92 PSE
93 PSE
94 PSE
95 GTO 03
96♦LBL 02
97 RCL 00
98 1/X
99 RCL 01
100 1/X
101 -
102 RCL 01
103 1/X
104 RCL 02
105 1/X
106 -
107 /
108 RCL 03
109 *
110 STO 05
111 RCL 03
112 +
113 STO 04
114 CLA
115 "F="
116 ARCL 04
117 AVIEW
118 PSE
119 PSE
120 PSE
121 CLA
122 "P="
123 ARCL 05
124 AVIEW
125 PSE
126 PSE
127 PSE
128♦LBL 03
129 RCL 01
130 RCL 02
131 -
132 RCL 00
133 RCL 02
134 -
135 /
136 RCL 06
137 RCL 00
138 -
139 RCL 06
140 RCL 01
141 -
142 /
143 *
144 STO 07
145 FIX 4
146 CLA
147 "THETA= "
148 ARCL 07
149 AVIEW
150 PSE
151 PSE
152 PSE
153 SF 02
154♦LBL 04
155 CLA
156 "HOW MANY SIZE F"
157 "⊢RACTIONS?"
158 PROMPT
159 1000
160 /
161 STO 48
162 STO 45
163 8
164 STO 46
165 20
166 STO 47
167 "ENTER OVERFLOW"
168 AVIEW
169 PSE
170 PSE
171♦LBL 05
172 ISG 45
173 GTO 06
174 GTO 07
175♦LBL 06
176 CLA
177 "ENTER dS, W"
178 PROMPT
179 ST+ 44
180 STO IND 47
181 RDN
182 STO IND 46
183 1
184 ST+ 46
185 ST+ 47
186 GTO 05
187♦LBL 07
188 RCL 48
189 STO 45
190 FS? 02
191 GTO 08
192 GTO 09
193♦LBL 08
194 20
195 STO 47
196 32
197 STO 46
198 GTO 10
199♦LBL 09
200 20
201 STO 46
202 STO 47
203♦LBL 10
204 ISG 45
205 GTO 11
206 GTO 12
207♦LBL 11
208 RCL IND 47
209 RCL 44
210 /
211 STO IND 46
212 1
213 ST+ 46
214 ST+ 47
215 GTO 10
216♦LBL 12
217 FC? 02
218 GTO 13
219 RCL 48
220 STO 45
221 "ENTER UNDERFLOW"
222 AVIEW
223 PSE
224 CF 02
225 0
226 STO 44
227 8
228 STO 46
229 20
230 STO 47
231 GTO 05
232♦LBL 13
233 RCL 48
234 .001
235 -
236 STO 45
237 21
238 STO 47
239 33
240 STO 46
241 8
242 STO 52
243♦LBL 14
244 ISG 45
245 GTO 15
246 GTO 16
247♦LBL 15
248 RCL 07
249 RCL IND 47
250 *
251 1
252 RCL 07
253 -
254 RCL IND 46
255 *
256 RCL 07
257 RCL IND 47
258 *
259 +
260 /
261 STO 51
262 RCL IND 52
263 STO 53
264 1
265 ST+ 52
266 RCL IND 52
267 RCL 53
268 +
```

Table I

```
269 2
270 /
271 STO IND 47
272 STO 53
273 "dT= "
274 ARCL 53
275 AVIEW
276 PSE
277 PSE
278 PSE
279 "T="
280 ARCL 51
281 AVIEW
282 PSE
283 PSE
284 PSE
285 1
286 ST+ 46
287 ST+ 47
288 GTO 14
289♦LBL 16
290 "PLOT CURVE"
291 PROMPT
292 CLA
293 "ENTER d50"
294 PROMPT
295 STO 49
296 9
297 STO 46
298 21
299 STO 47
300 RCL 48
301 .001
302 -
303 STO 45
304 RCL 08
305 STO 51
306 XEQ E
307 GTO 17
308♦LBL E
309 RCL 49
310 /
311 .115
312 -
313 3
314 Y↑X
315 CHS
316 E↑X
317 CHS
318 1
319 +
320 100
321 *
322 STO 53
323 CLA
324 "d="
325 ARCL 51
326 AVIEW
327 PSE
328 PSE
329 PSE
330 CLA
331 "E="
332 ARCL 53
333 AVIEW
334 PSE
335 PSE
336 PSE
337 RTN
338♦LBL 17
339 ISG 45
340 GTO 18
341 GTO 19
342♦LBL 18
343 RCL IND 47
344 STO 51
345 XEQ E
346 RCL IND 46
347 STO 51
348 XEQ E
349 1
350 ST+ 46
351 ST+ 47
352 GTO 17
353♦LBL 19
354 25
355 STO 51
356 XEQ F
357 STO 54
358 "d25= "
359 ARCL 54
360 AVIEW
361 PSE
362 PSE
363 PSE
364 75
365 STO 51
366 XEQ F
367 STO 51
368 "d75= "
369 ARCL 51
370 AVIEW
371 PSE
372 PSE
373 PSE
374 RCL 51
375 RCL 54
376 -
377 2
378 RCL 49
379 *
380 /
381 STO 53
382 "I= "
383 ARCL 53
384 PROMPT
385♦LBL F
386 RCL 51
387 100
388 /
389 CHS
390 1
391 +
392 LN
393 CHS
394 .3333
395 Y↑X
396 .115
397 +
398 RCL 49
399 *
400 RTN
401 .END.
```

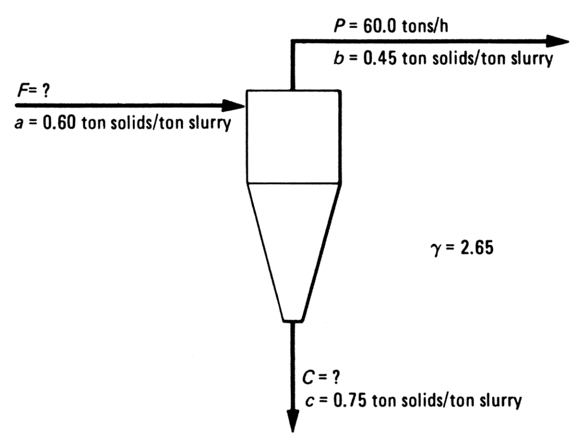
HP-41C memory map for hydrocyclone program — Table II

Register	Contents
00	c
01	a
02	b
03	C
04	F
05	P
06	γ
07	Θ
08 – 19	d_i, $i = 1 - 12$
20 – 31	(1) W_i, $i = 1 - 12$ (2) R_{a_i}, $i = 1 - 12$ (3) d_{T_i}, $i = 1 - 12$
32 – 43	R_{c_i}, $i = 1 - 12$
44	W
45	ISG index
46	Indirect address #1
47	Indirect address #2
48	Total number of size fractions/1000
49	d_{50}
50	T_i
51	Used
52	Indirect address #3
53	(1) E (2) I
54	d_{25}

Data for sample problem — Table III

100 gram screen analysis

Screen size (microns) d_S	Weights solids retained on each screen (grams) W: Overflow	Underflow
250	0.0	5.0
200	0.0	10.0
150	5.0	20.0
100	55.0	40.0
50	15.0	10.0
0	25.0	15.0



Entering the data for sample problem — **Table IV**

1. Clear memory.
2. Execute the calculator SIZE function for 55 registers.
3. Load the program into the calculator.

To begin execution, set the calculator to USER mode, and press the "A" button. Execution will proceed as follows. (Note: Underlined items indicate calculator output, and non-numerical operations are indicated in parentheses.)

Enter C, c, P
0 (Enter) 0.75
(Enter) 60 (R/S)
[Note: For C, F, and P, enter the value for the one known. 0 is entered for the two unknown values.]

Enter b, F, a
0.45 (Enter) 0
(Enter) 0.60 (R/S)
Enter γ
2.65 (R/S)
C=100.0
F=160.0
Θ = 0.4634
How many size fractions?
6 (R/S)
Enter overflow
Enter ds, W
250 (Enter) 0.0 (R/S)
Enter ds, W
200 (Enter) 0.0 (R/S)
Enter ds, W
150 (Enter) 5.0 (R/S)
Enter ds, W
100 (Enter) 55.0 (R/S)
Enter ds, W
50 (Enter) 15.0 (R/S)
Enter ds, W
0 (Enter) 25.0 (R/S)
Enter underflow

Enter ds, W
250 (Enter) 5.0 (R/S)
Enter ds, W
200 (Enter) 10.0 (R/S)
Enter ds, W
150 (Enter) 20.0 (R/S)
Enter ds, W
100 (Enter) 40.0 (R/S)
Enter ds, W
50 (Enter) 10.0 (R/S)
Enter ds, W
0 (Enter) 15.0 (R/S)
dT=225.0
T=1.0
dT=175.0
T=0.7755
dT=125.0
T=0.3858
dT=75.0
T=0.3654
dT=25.0
T=0.3413
Plot curve

[Note: At this time it is necessary to plot the Tromp curve and determine d_{50} (see Fig. 9). When this is done, proceed with the remainder of the program. For this example, d_{50} was determined to be approximately 152 microns.]

Enter d 50
152.0 (R/S)
d=250.0
E=97.2117
d=225.0
E=92.1509
d=200.0
E=82.2966
d=175.0
E=67.1412
d=150.0
E=48.4540
d=125.0
E=29.8087
d=100.0
E=14.7865
d=75.0
E=5.2749
d=50.0
E=0.9745
d=25.0
E=0.0121
d=0.0
E=−0.1522
d 25=117.8258
d 75=186.9622
I=0.2274

[Note: This is the final output in the execution of the program.]

d_{50} value. When this is accomplished, restart the program, and enter the d_{50} value. The calculator will now output the efficiencies for each screen size, as well as the mean size for each size fraction, using Eq. (5). Next, it will output d_{25} and d_{75} values, using Eq. (6), and then with these values will determine the imperfection number by means of Eq. (7). This number is output, and program execution ends. The flowchart for this program is shown in Fig. 8. The program listing is in Table I, and the memory map is shown in Table II, on p. 77.

Sample problem

Table III defines a situation that might be encountered in a mineral processing operation. The tonnage in the hydrocyclone overflow is known, along with the solids contents of the three slurries and the specific gravity of the solid material. The operator wishes to determine how efficiently the system is operating over the range of particle sizes involved. To do this, screen tests have been run on 100-gram samples of the solid material in the overflow and underflow, with the results shown below the diagram. The use of the program is demonstrated in Table IV.

Limitations of the program

From the example problem, it will be noticed that, although six sets of size fraction data were entered, only five Tromp values were generated. The Tromp value for the +250-micron material cannot be generated with this program unless a set of "dummy" data is entered first. Such a data set for the example just given would require a particle size greater than 250 microns, and a very small, yet finite weight. This dummy set would be treated as the first size fraction to be entered, and the total number of size fractions would be increased from six to seven. In the example above, if the dummy set were used, the calculator would be told that there are seven size fractions to be entered, and the dummy data would be the first data set entered for both the overflow and the underflow. In this example, a data set of $d_s = 300.0$, $W = 0.001$ would result in the Tromp value for the +250-micron size fraction being generated and displayed. At the same time, the dummy data will have no effect on the accuracies of the numbers calculated for the true data subsequently entered.

Another limitation concerns the total number of size fractions the program can handle. As written, the program is limited to twelve sets of size fraction data for each of the overflow and the underflow. Should it be desired to work with more data sets, the program can be reworked to accommodate additional sets within the limits of available calculator memory. The modification involves increasing the number of registers allocated to memory in the calculator, repositioning the information contained in registers 44 through 54, and expanding the number of registers contained in each of the three sets of registers 8 − 19, 20 − 31, and 32 − 43. The program can also be modified to print out all results on the HP-82143A printer.

Comments*

Sir: There are a couple of points in your article "Program calculates hydrocyclone efficiency" that require some comment. The overall mass recovery by the cyclone has been computed by the use of percent solids in the cyclone feed. I submit that while this would be acceptable, it is an almost impossible number to obtain directly. A sample taken upstream of the pump feeding the cyclone does not account for water maintaining the sump level or gland water. Personal experience has shown that reliable samples are impossible to get from the feed line. Therefore, one is forced to rely on screen data to compute the Tromp value. The equation is:

$$T_i = \left(\frac{P_i}{F_i}\right)\left(\frac{F_i - C_i}{P_i - C_i}\right), \text{ or } T_i = \left(\frac{F_i}{P_i}\right)\theta$$

where θ is some averaged value for the mass recovery and the other symbols are as defined in the article.

Now note that as the d_{50} size is approached, P_i and C_i are going to become approximately equal. The reliability of the data is very shaky because the equation requires division by the difference between two large (relative) numbers.

If the θ value is used, the data are smeared through-

*Letter originally published June 14, 1982.

out the rest of the curve and distort the two knees, which are the most valuable area of the curves. It is better to plot the data and then interpolate to the d_{50} value.

One further point: for the Tromp curves shown, the fines tail does not approach the lower axis as one would expect. This is because a fraction of the ore is not classified in the cyclone but passes from the inlet directly out the apex (underflow). This fraction is equal to the fraction of water that exits the underflow. If it is important to remove these fines from the underflow, there are corrective actions that can be taken.

R. L. ATWOOD
Chief Metallurgist
Foote Mineral Co.

Author replies

Dr. Atwood is quite correct when he states that the percent solids in the cyclone feed is almost an impossible number to obtain directly. Early in my work with cyclones, I found that the best method to obtain a good estimate of this value was to calculate it from the volumetric feed rate to the cyclone and the solids contents of the overflow and underflow streams.

The procedure for doing this is to use a Doppler-type flowmeter to take flowrates from the cyclone feed line. Samples of both the overflow and underflow are taken and weighed in a Marcy pulp scale. This provides the solids contents and the specific gravities of the overflow and underflow. From this information, along with the solids feed rate to the system (weight solids in the overflow), the percent solids in the cyclone feed stream can be calculated.

Should a flowmeter not be available for determining the feed flowrate, Dr. Atwood's procedure, however, is the only available method for calculating T_i without the necessity of going to great lengths.

I appreciate Dr. Atwood's bringing this matter to my attention. This problem was not addressed in the paper, and definitely should have been.

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For TI-58/59 users

The version of the program for TI users appears in Table V. For the Texas Instruments calculators, the memory of the device alone is large enough to accommodate the program, data storage and calculations. User instructions appear in Table VI. The data input and the output tape for the sample problem are presented in Table VII, to ensure that the user instructions are clear to the reader. The same problem that was used for the HP version is run—see Table III.

Program listing for TI version **Table V**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	034	23	LNX	068	24	CE	102	95	=	136	05	05
001	11	A	035	53	(	069	76	LBL	103	42	STO	137	85	+
002	42	STO	036	43	RCL	070	22	INV	104	03	03	138	43	RCL
003	04	04	037	01	01	071	22	INV	105	61	GTO	139	03	03
004	91	R/S	038	35	1/X	072	86	STF	106	24	CE	140	95	=
005	76	LBL	039	75	-	073	00	00	107	76	LBL	141	42	STO
006	12	B	040	43	RCL	074	53	(	108	23	LNX	142	04	04
007	86	STF	041	00	00	075	43	RCL	109	22	INV	143	76	LBL
008	01	01	042	35	1/X	076	02	02	110	86	STF	144	24	CE
009	42	STO	043	54	)	077	35	1/X	111	01	01	145	43	RCL
010	03	03	044	55	÷	078	75	-	112	53	(	146	04	04
011	91	R/S	045	53	(	079	43	RCL	113	43	RCL	147	99	PRT
012	76	LBL	046	43	RCL	080	00	00	114	00	00	148	43	RCL
013	13	C	047	02	02	081	35	1/X	115	35	1/X	149	03	03
014	86	STF	048	35	1/X	082	54	)	116	75	-	150	99	PRT
015	00	00	049	75	-	083	55	÷	117	43	RCL	151	43	RCL
016	42	STO	050	43	RCL	084	53	(	118	01	01	152	05	05
017	05	05	051	00	00	085	43	RCL	119	35	1/X	153	99	PRT
018	91	R/S	052	35	1/X	086	01	01	120	54	)	154	98	ADV
019	76	LBL	053	54	)	087	35	1/X	121	55	÷	155	91	R/S
020	14	D	054	65	×	088	75	-	122	53	(	156	42	STO
021	42	STO	055	43	RCL	089	43	RCL	123	43	RCL	157	06	06
022	01	01	056	04	04	090	00	00	124	01	01	158	53	(
023	91	R/S	057	95	=	091	35	1/X	125	35	1/X	159	43	RCL
024	42	STO	058	42	STO	092	54	)	126	75	-	160	01	01
025	00	00	059	05	05	093	65	×	127	43	RCL	161	75	-
026	91	R/S	060	94	+/-	094	43	RCL	128	02	02	162	43	RCL
027	42	STO	061	85	+	095	05	05	129	35	1/X	163	02	02
028	02	02	062	43	RCL	096	95	=	130	54	)	164	54	)
029	87	IFF	063	04	04	097	42	STO	131	65	×	165	55	÷
030	00	00	064	95	=	098	04	04	132	43	RCL	166	53	(
031	22	INV	065	42	STO	099	75	-	133	03	03	167	43	RCL
032	87	IFF	066	03	03	100	43	RCL	134	95	=	168	00	00
033	01	01	067	61	GTO	101	05	05	135	42	STO	169	75	-

(Continued) Table V

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
170	43	RCL	225	09	9	280	95	=	335	59	59	390	02	2
171	02	02	226	42	STO	281	99	PRT	336	85	+	391	05	5
172	54	)	227	58	58	282	98	ADV	337	09	9	392	42	STO
173	65	×	228	76	LBL	283	43	RCL	338	95	=	393	56	56
174	53	(	229	35	1/X	284	58	58	339	67	EQ	394	71	SBR
175	43	RCL	230	73	RC*	285	32	X↕T	340	52	EE	395	53	(
176	06	06	231	58	58	286	43	RCL	341	61	GTO	396	42	STO
177	75	−	232	32	X↕T	287	59	59	342	43	RCL	397	55	55
178	43	RCL	233	03	3	288	65	×	343	76	LBL	398	93	.
179	00	00	234	44	SUM	289	03	3	344	52	EE	399	07	7
180	54	)	235	58	58	290	85	+	345	86	STF	400	05	5
181	55	÷	236	73	RC*	291	08	8	346	01	01	401	42	STO
182	53	(	237	58	58	292	95	=	347	61	GTO	402	56	56
183	43	RCL	238	85	+	293	67	EQ	348	43	RCL	403	71	SBR
184	06	06	239	32	X↕T	294	34	$\sqrt{X}$	349	76	LBL	404	53	(
185	75	−	240	95	=	295	02	2	350	42	STO	405	75	−
186	43	RCL	241	55	÷	296	22	INV	351	32	X↕T	406	43	RCL
187	01	01	242	02	2	297	44	SUM	352	93	.	407	55	55
188	54	)	243	95	=	298	58	58	353	01	1	408	95	=
189	95	=	244	99	PRT	299	61	GTO	354	01	1	409	55	÷
190	42	STO	245	01	1	300	35	1/X	355	05	5	410	02	2
191	07	07	246	44	SUM	301	76	LBL	356	77	GE	411	55	÷
192	99	PRT	247	58	58	302	34	$\sqrt{X}$	357	45	Y^x	412	43	RCL
193	98	ADV	248	73	RC*	303	91	R/S	358	32	X↕T	413	57	57
194	09	9	249	58	58	304	42	STO	359	99	PRT	414	95	=
195	42	STO	250	65	×	305	57	57	360	55	÷	415	99	PRT
196	58	58	251	53	(	306	09	9	361	43	RCL	416	98	ADV
197	91	R/S	252	43	RCL	307	42	STO	362	57	57	417	91	R/S
198	42	STO	253	07	07	308	58	58	363	75	−	418	76	LBL
199	59	59	254	94	+/−	309	76	LBL	364	93	.	419	53	(
200	91	R/S	255	85	+	310	43	RCL	365	01	1	420	99	PRT
201	76	LBL	256	01	1	311	73	RC*	366	01	1	421	94	+/−
202	32	X↕T	257	54	)	312	58	58	367	05	5	422	85	+
203	72	ST*	258	95	=	313	71	SBR	368	95	=	423	01	1
204	58	58	259	32	X↕T	314	42	STO	369	45	Y^x	424	95	=
205	01	1	260	01	1	315	73	RC*	370	03	3	425	23	LNX
206	44	SUM	261	44	SUM	316	58	58	371	95	=	426	94	+/−
207	58	58	262	58	58	317	32	X↕T	372	94	+/−	427	45	Y^x
208	43	RCL	263	73	RC*	318	03	3	373	22	INV	428	53	(
209	58	58	264	58	58	319	44	SUM	374	23	LNX	429	01	1
210	32	X↕T	265	65	×	320	58	58	375	94	+/−	430	55	÷
211	43	RCL	266	43	RCL	321	73	RC*	376	85	+	431	03	3
212	59	59	267	07	07	322	58	58	377	01	1	432	54	)
213	65	×	268	95	=	323	85	+	378	95	=	433	85	+
214	03	3	269	42	STO	324	32	X↕T	379	65	×	434	93	.
215	85	+	270	57	57	325	95	=	380	01	1	435	01	1
216	09	9	271	32	X↕T	326	55	÷	381	00	0	436	01	1
217	95	=	272	85	+	327	02	2	382	00	0	437	05	5
218	67	EQ	273	43	RCL	328	95	=	383	95	=	438	95	=
219	33	X^2	274	57	57	329	71	SBR	384	99	PRT	439	65	×
220	91	R/S	275	95	=	330	42	STO	385	98	ADV	440	43	RCL
221	61	GTO	276	35	1/X	331	43	RCL	386	92	RTN	441	57	57
222	32	X↕T	277	65	×	332	58	58	387	76	LBL	442	95	=
223	76	LBL	278	43	RCL	333	32	X↕T	388	45	Y^x	443	99	PRT
224	33	X^2	279	57	57	334	43	RCL	389	93	.	444	98	ADV
												445	92	RTN

User instructions for TI version **Table VI**

Step		Value	Key or output
1.	Enter one of three flowrates in tons solids/h:		
	Hydrocyclone feed	F	Press **A**
	or hydrocyclone underflow	C	Press **B**
	or hydrocyclone overflow	P	Press **C**
2.	Enter all of the following solids contents in tons solids/ton slurry:		
	Solids content of feed	a	Press **D**
	Solids content of underflow	c	Press **R/S**
	Solids content of overflow	b	Press **R/S**
3.	Program will calculate and print:		
	Feed, tons solids/h		F
	Underflow, tons solids/h		C
	Overflow, tons solids/h		P
4.	Enter specific gravity of solids	γ	Press **R/S**
5.	Program will calculate and print:		
	Overall mass recovery		θ
6.	Enter screening data:		
	Number of screens, n	n	Press **R/S**
	For each screen:		
	Screen size, μm	d_s	Press **R/S**
	Overflow, wt.% retained on screen	W_{over}	Press **R/S**
	Underflow, wt.% retained on screen	W_{under}	Press **R/S**
	(Program will display "27" after each of the above entries.)		
7.	When all screen data are entered, program calculates data for Tromp curve:		
	Midpoint between screen sizes, μm		dT
	Tromp value		T
8.	Plot these data; T vs. size, and locate the d_{50} value, the size for $T = 0.50$		
	Enter the size for $T = 0.50$, μm	d_{50}	Press **R/S**
9.	Machine will calculate and print:		
	Particle size, μm		d
	Hydrocyclone efficiency for that size		E
	This will be done for each screen and for the midpoint between screen sizes.		
	The zero size with negative efficiency will not be included in this output.		
	The 25% and 75% efficiency sizes		0.25
			d_{25}
			0.75
			d_{75}
	Imperfection value		I

Example for the TI version **Table VII**

Step		Value	Key or output	
1.	Enter hydrocyclone underflow	60	Press **A**	
2.	Enter solids contents:			
	Feed	0.60	Press **D**	
	Underflow	0.75	Press **R/S**	
	Overflow	0.45	Press **R/S**	
3.	Program calculates and prints:			
	Feed			160.
	Underflow			100.
	Overflow			60.
4.	Enter specific gravity of solids	2.64	Press **R/S**	
5.	Program calculates and prints:			
	Overall mass recovery		.4632352941	

(Continued) Table VII

Step	Instructions	Input	Keys	Output
6.	Enter screening data:			
	Number of screens	6	Press **R/S**	
	Screen size, overflow, underflow for each screen:		250 **R/S** 0 **R/S** 5 **R/S**	
			200 **R/S** 0 **R/S** 10 **R/S**	
			150 **R/S** 5 **R/S** 20 **R/S**	
			100 **R/S** 55 **R/S** 40 **R/S**	
			50 **R/S** 15 **R/S** 10 **R/S**	
			0 **R/S** 25 **R/S** 15 **R/S**	
7.	Program calculates and prints:			
	Midpoint between screen sizes			225.
	Tromp value			1.
8.	Plot data. The size is 152. Enter it:	152	Press **R/S**	
9.	Program calculates and prints:			
	Particle size			175.
	Hydrocyclone efficiency for that size			.7753846154
	Particle size			125.
	Hydrocyclone efficiency for that size			.3856159143
	Particle size			75.
	Hydrocyclone efficiency for that size			.3652173913
	Particle size			25.
	Hydrocyclone efficiency for that size			.3411552347
	Particle size			250.
	Hydrocyclone efficiency for that size			97.21167531
	Particle size			225.
	Hydrocyclone efficiency for that size			92.15091621
	Particle size			200.
	Hydrocyclone efficiency for that size			82.29658754
	Particle size			175.
	Hydrocyclone efficiency for that size			67.14123878
	Particle size			150.
	Hydrocyclone efficiency for that size			48.45395661
	Particle size			125.
	Hydrocyclone efficiency for that size			29.80871273
	Particle size			100.
	Hydrocyclone efficiency for that size			14.78646599
	Particle size			75.
	Hydrocyclone efficiency for that size			5.274868246
	Particle size			50.
	Hydrocyclone efficiency for that size			.9745318435
	Particle size			25.
	Hydrocyclone efficiency for that size			.0121086707
	The 25 and 75% efficiency sizes			0.25
				117.8216383
				0.75
				186.9640136
	Imperfection value			.2274420242

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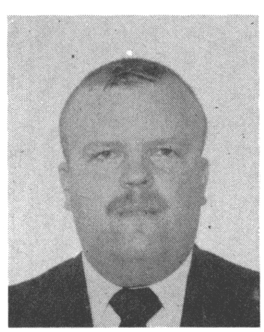

The author

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Program performs vapor-liquid equilibrium calculations

The dewpoint, bubble point and equilibrium flash are easily obtainable with this program, written for the HP-41CV, or 41C with a quad memory module.

Victor L. Rice, Oklahoma State University

☐ Here we will present a program for the Hewlett-Packard HP-41CV or 41C calculators that solves basic vapor-liquid equilibrium problems—calculation of the dewpoint, bubble point, and equilibrium flash. The algorithm employed uses a method for predicting ideal-solution *K*-values developed by Edmister [*1*]. To better understand this method, a brief review of some vapor-liquid equilibrium fundamentals is presented. Following this, a description of the calculator program and an example will be given.

Vapor-liquid equilibrium

To perform the three vapor-liquid equilibrium calculations one must determine the *K*-value for each component. The accuracy in estimating this quantity will establish the accuracy of the final result. The *K*-value can be defined as follows:

$$K_i \equiv \frac{y_i}{x_i} = \left(\frac{\phi_i^L}{\phi_i^V}\right)\left(\frac{\gamma_i^L}{\gamma_i^V}\right) \qquad (1)$$

The vapor-phase functions (ϕ_i^V, γ_i^V) can be obtained from any applicable equation of state via the following:

$$\ln \phi_i^V = \frac{1}{RT}\int_0^P \left(\underline{V}_i{}^V - \frac{RT}{P}\right) \mathrm{d}P \qquad (2)$$

$$\ln \gamma_i^V = \frac{1}{RT}\int_0^P \left(\bar{V}_i^V - \underline{V}_i^V\right) \mathrm{d}P \qquad (3)$$

Eq. (2) and (3) are general and could also apply to the liquid phase. But for this to be true, the equation of state for the vapor phase should also be able to predict liquid volumetric properties.

Although equations of state generally will not adequately predict liquid properties, a few (e.g., those of Soave-Redlich-Kwong, and Peng-Robinson) allow fairly accurate prediction. Unfortunately, their applicability is restricted to systems of "normal fluids," such as the rare gases, nitrogen, oxygen, carbon monoxide and hydrocarbons [*2*]. Also included are carbon dioxide, hydrogen, hydrogen sulfide, and, with certain limitations, some slightly polar substances. For more-complex systems, the liquid activity-coefficient model approach must be used. This method requires experimental equilibrium data.

Developing K_i

Eq. (2) can be manipulated so as to allow the prediction of ϕ_i^L from existing equations of state. When integrating Eq. (2) (for the liquid phase) one must account for the phase change from vapor to liquid. Due to the discontinuity of the molal volume at the phase transition, the integration has to be done in three steps (all at constant temperature):

Step 1: $0 \rightarrow p_i^0$ Vapor
Step 2: At p_i^0 Vapor to liquid
Step 3: $p_i^0 \rightarrow P$ Liquid

Since Step 1 is for the vapor phase, Eq. (2) can be used with an equation of state to predict the volume term. The upper integration limit would be p_i^0. The change in ϕ_i^L for Step 2 is zero. The change in ϕ_i^L for Step 3 is:

$$\ln \phi_i^L = \frac{1}{RT}\int_{p_i^0}^P \left(\underline{V}_i^L - \frac{RT}{P}\right) \mathrm{d}P = \frac{1}{RT}\int_{p_i^0}^P \underline{V}_i^L\, \mathrm{d}P + \ln\left(\frac{p_i^0}{P}\right) \qquad (4)$$

Thus, the sum of the three steps yields:

$$\ln \phi_i^L = \frac{1}{RT}\int_0^{p_i^0} \left(\underline{V}_i^V - \frac{RT}{P}\right) \mathrm{d}P + \frac{1}{RT}\int_{p_i^0}^P \underline{V}_i^L\, \mathrm{d}P + \ln\left(\frac{p_i^0}{P}\right) \qquad (5)$$

Eq. (1) becomes:

$$K_i = \left(\frac{p_i^0}{P}\right)\left(\frac{\gamma_i^L}{\gamma_i^V}\right) \exp\left[\frac{1}{RT}\int_{p_i^0}^P V_i^L\, \mathrm{d}P\right] \times \exp\left[\frac{1}{RT}\int_P^{p_i^0} \left(\underline{V}_i^V - \frac{RT}{P}\right) \mathrm{d}P\right] \qquad (6)$$

The last term in Eq. (6) results from the combination of the first term in Eq. (5) with Eq. (2) for ϕ_i^V. Eq. (6) is

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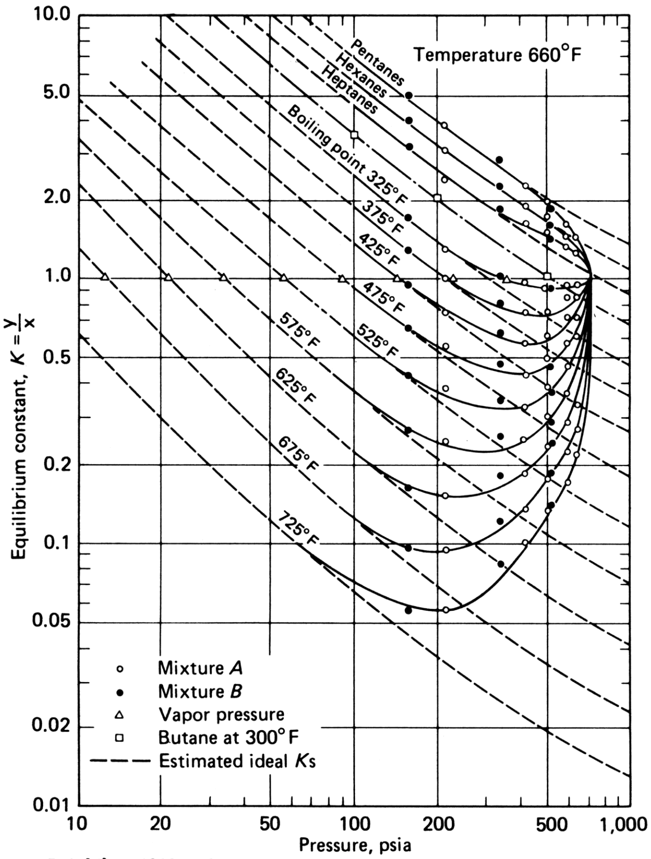


Source: Ref. [4]. ©1963 McGraw-Hill. Used with permission of publisher.

K values are closer to ideal ones for smaller molecules at lower pressures **Fig. 1**

Constants used in Eq. (7) through (14) **Table I**

Constant	$P_r < 1.0$	$1.0 < P_r < 10.0$	$P_r > 10.0$
For $K_R < 1.0$			
a_0	+0.72354688	+0.71613974	+0.93322546
a_1	−0.11955262	−0.11010362	−0.29838149
a_2	−0.019175521	−0.009820518	+0.036108945
a_3	−0.00079043357	+0.00085139636	−0.0018123488
a_4	−0.092938874	−0.031743583	−1.4698873
a_5	−0.089253134	−0.077912651	+1.5375645
a_6	−0.02120992	−0.012739586	−0.71906421
a_7	−0.0011023254	−0.035998746	+0.089098628
a_8	+0.83485814	+3.4719935	−0.33924284
a_9	−1.7510463	−2.4128931	+1.3802654
a_{10}	−1.7882516	+0.74548583	−0.64746142
a_{11}	−0.20255145	−0.13713069	+0.074000484
For $K_R > 1.0$			
a_{12}	+0.55823912	+0.56319800	+0.3986012
a_{13}	−0.22417339	−0.20762898	−0.1933524
a_{14}	−0.026665354	−0.001581164	+0.02388513
a_{15}	−0.0046116207	−0.0001901561	+0.17430118
a_{16}	+0.035372461	+0.023954299	−0.082957315
a_{17}	+0.0067313403	−0.00380481	+0.010571085
a_{18}	−0.00060208161	−0.0017300384	−0.032969708
a_{19}	−0.002218345	−0.0022414988	+0.021278044
a_{20}	−0.0004783554	+0.0013698449	−0.0032276668

Source: Edmister [1].

rigorous and is based on the First Law and Second Law. The first term in Eq. (6), $\frac{p_i^0}{P}$, is known as Raoult's Law K-value (K_R), which is valid only for completely ideal systems. Thus, K_i as given in Eq. (6) can be viewed as Raoult's Law K-value with four corrections:

1. Effect of molecular interactions in the liquid phase, γ_i^L.
2. Effect of molecular interactions in the vapor phase, γ_i^V.
3. Pure-component nonideality in the liquid phase, the third term.
4. Pure-component nonideality in the vapor phase, the fourth term.

Several assumptions can be made regarding Eq. (6) that simplify, to varying degrees, the calculation of K_i. Of course, these assumptions limit the applicability of the equation. Fair and Bolles [5] list such assumptions and show how they limit applicability.

In developing his correlation for ideal-solution K-values, Edmister assumed ideal liquid and vapor solutions, and that the liquid is incompressible. The ideal-solution model is a very good approximation for close-boiling homologs, but is not for other systems [3]. The applicability of assuming an ideal solution depends upon the degree of accuracy desired, as well as the molecular structure of the components.

Fig. 1 illustrates the deviation from reality of the ideal-solution model. The actual components shown in Fig. 1 are not as important as is their behavior in regard to K_i. As molecules become more complex, the deviation of the ideal-solution K-values from the experimental ones becomes significant at lower pressures.

Fig. 1 is for hydrocarbon mixtures, as well as for pure hydrocarbons. The lower lines in the figure are for boiling-point fractions. Mixtures A and B are hydrocarbon mixtures. The higher-boiling-point mixtures are made up of a large range of molecular-weight materials. Such a range is a factor in K's deviation from ideality.

This figure illustrates the need for judgment in applying this model. Assuming that the liquid is incompressible is generally true at normal pressures. Thus, this assumption does not introduce any significant error.

Edmister's book should be consulted for how he developed his correlation. His K-values are the ones used in the program. The end-result is:

For $K_R < 1.0$:

$$Y = A_0X + A_1[(1 + A_2X)e^{X/2} - 1] \quad (7)$$

$$A_0 = a_0 + a_1Z + a_2Z^2 + a_3Z^3 \quad (8)$$

$$A_1 = a_4 + a_5Z + a_6Z^2 + a_7Z^3 \quad (9)$$

$$A_2 = a_8 + a_9Z + a_{10}Z^2 + a_{11}Z^3 \quad (10)$$

For $K_R > 1.0$:

$$Y = A_3X + A_4X^2 + A_5X^3 \quad (11)$$

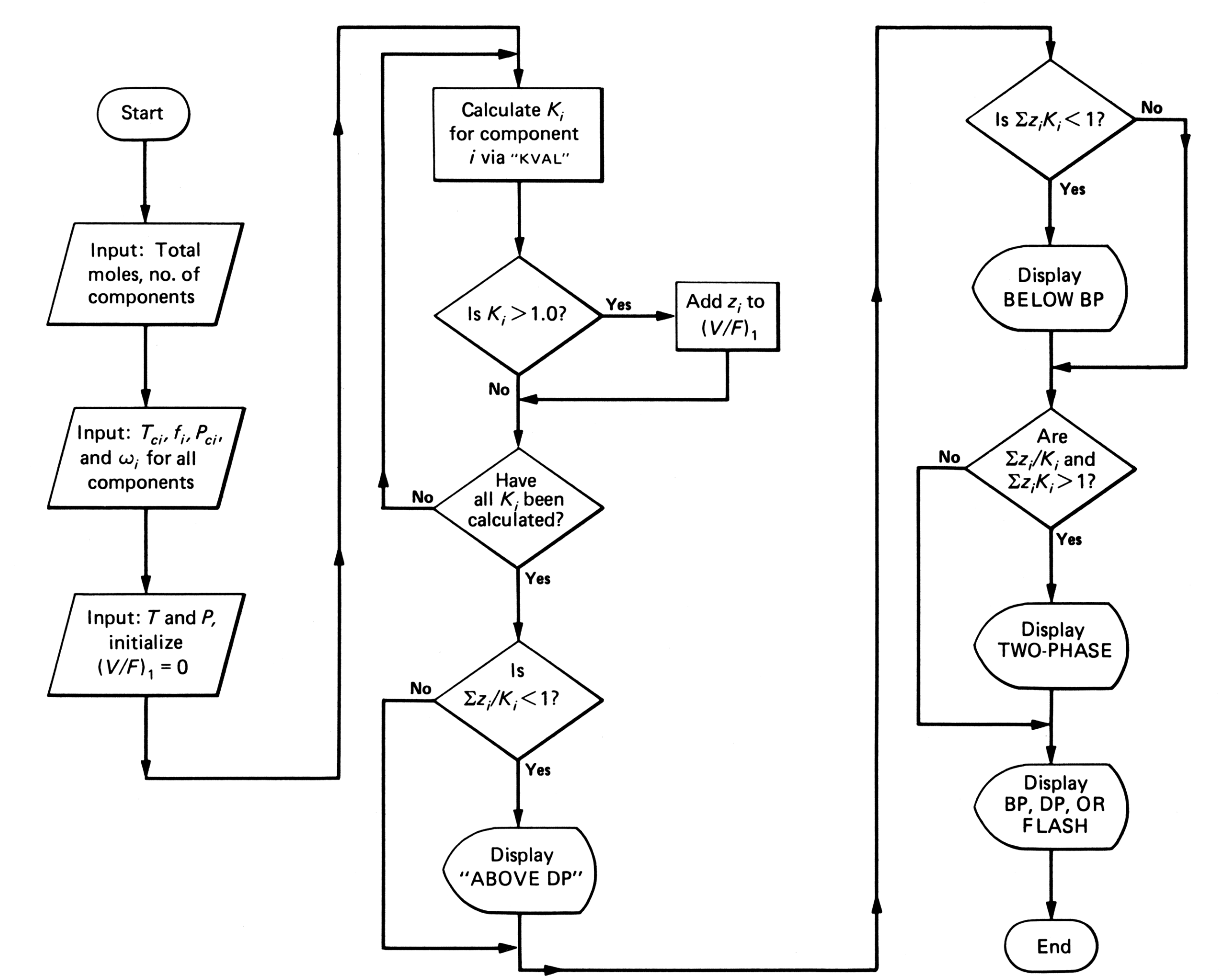
$$A_3 = a_{12} + a_{13}Z + a_{14}Z^2 \quad (12)$$

$$A_4 = a_{15} + a_{16}Z + a_{17}Z^2 \quad (13)$$

$$A_5 = a_{18} + a_{19}Z + a_{20}Z^2 \quad (14)$$

where $$Y = \ln K_I \quad (15)$$

(Text continues on p. 224)



Here the program determines and displays certain basic information **Fig. 2**

Nomenclature

- A see Eq. (7) to (14)
- a see Eq. (7) to (14)
- F feedrate, lb-mol/h
- f feedrate of component i, lb-mol/h
- K equilibrium distribution coefficient
- K_I ideal-solution K-value, Eq. (15)
- K_R Raoult's Law K-value
- l rate of component i in liquid product, lb-mol/h
- N number of components in feed
- p^0 pure-component vapor pressure, psia
- P pressure, psia
- R gas constant
- S convergence function
- T temperature, °F (or R)
- v rate of component i in vapor product, lb-mol/h
- V total vapor rate, lb-mol/h
- $\overline{V}$ partial molal volume, ft^3/lb-mol
- $\underline{V}$ molal volume, ft^3/lb-mol
- X as defined in Eq. (16)
- x liquid mole fraction
- Y as defined in Eq. (15)
- y vapor mole fraction
- Z as defined in Eq. (17)
- z feed mole fraction

Greek letters

- γ activity coefficient
- ϕ fugacity coefficient
- ω acentric factor

Subscripts

- c critical property
- i component i property or quantity
- k counter of trial-and-error loop in flash calculation
- r reduced property
- bp bubble point
- dp dewpoint

Superscripts

Letters:

- V vapor property
- L liquid property

Numbers:

- 0 for a pure component

Program performs vapor-liquid equilibrium calculations for the HP-41C calculator

```
01♦LBL "VLE"
```

Component data input

```
02 ADV
03 "VAPOR-LIQUID EQ"
04 "⊢UILIBRIUM"
05 FS? 21
06 PRA
07 ADV
08 "TOT MOLES=?"
09 PROMPT
10 STO 78
11 "N=?"
12 PROMPT
13 STO 00
14 "TC UNITS=?"
15 AON
16 PROMPT
17 ASTO Y
18 AOFF
19 "F"
20 ASTO X
21 X=Y?
22 SF 07
23 CLA
24 XEQ 15
25♦LBL 06
26 RCL 81
27 FIX 0
28 CF 29
29 ARCL X
30 ASTO 83
31 459.67
32 SF 29
33 "TC"
34 ARCL 83
35 "⊢=?"
36 PROMPT
37 FS? 07
38 +
39 RND
40 "F"
41 ARCL 83
42 "⊢=?"
43 PROMPT
44 RCL 78
45 /
46 +
47 RCL 81
48 90
49 +
50 X<>Y
51 STO IND Y
52 "PC"
53 ARCL 83
54 "⊢=?"
55 PROMPT
56 RND
57 "OMEGA"
58 ARCL 83
59 "⊢=?"
60 PROMPT
61 +
62 RCL 81
63 100
64 +
65 X<>Y
66 STO IND Y
67 CLA
68 FIX 3
69 ISG 81
70 GTO 06
```

Input T and P

```
71♦LBL E
72 ADV
73 "**"
74 FS? 21
75 PRA
76 0
77 STO 77
78 "T=?, DEG F"
79 PROMPT
80 459.67
81 +
82 STO 84
83 "P=?"
84 PROMPT
85 STO 85
86 XEQ 15
```

Calculate and display K_i. If $K_i > 1.0$, add z_i to $(V/F)_1$

```
87♦LBL 00
88 XEQ "KVAL"
89 RCL 81
90 FIX 0
91 CF 29
92 "K"
93 ARCL X
94 "⊢="
95 RDN
96 FIX 4
97 SF 29
98 ARCL X
99 AVIEW
100 RCL 81
101 110
102 +
103 X<>Y
104 STO IND Y
105 1
106 X>Y?
107 GTO 05
108 XEQ 16
109 FRC
110 ST+ 77
```

Determines system phase

```
111♦LBL 05
112 ISG 81
113 GTO 00
114 0
115 STO 76
116 STO 82
117 SF 05
118 CF 06
119 XEQ 02
120 RCL 82
121 STO 90
122 "**ABOVE DP**"
123 1
124 X>Y?
125 AVIEW
126 X>Y?
127 SF 10
128 0
129 STO 82
130 SF 06
131 CF 05
132 XEQ 02
133 RCL 82
134 STO 88
135 "**BELOW BP**"
136 1
137 X>Y?
138 AVIEW
139 X>Y?
140 SF 10
141 PSE
142 "*TWO PHASE*"
143 FC?C 10
144 AVIEW
145 STOP
146♦LBL 02
147 XEQ 15
```

Calculates $\Sigma z_i K_i$ or $\Sigma z_i / K_i$

```
148♦LBL d
149 XEQ 16
150 FRC
151 XEQ 14
152 FS? 05
153 /
154 FS? 06
155 *
156 ST+ 82
157 ISG 81
158 GTO d
159 CF 05
160 CF 06
161 RTN
```

First flash trial

```
162♦LBL C
163 XEQ 15
164 CLX
165 XEQ 13
166 STO 79
167 X<0?
168 SF 02
169 RCL 77
170 STO 76
171 .05
172 FS?C 02
173 CHS
174 ST+ 77
```

Checks for convergence

```
175♦LBL 03
176 XEQ 15
177 CLX
178 XEQ 13
179 STO 80
180 "S="
181 ARCL X
182 AVIEW
183 PSE
184 CLD
185 ABS
186 1 E-05
187 X>Y?
188 GTO 02
189 RCL 76
190 CHS
191 RCL 77
192 STO 76
193 +
194 RCL 80
195 RCL 79
196 -
197 /
198 RCL 80
199 *
200 CHS
201 RCL 77
202 +
203 STO 77
204 RCL 80
205 STO 79
206 GTO 03
```

Summarizes output

```
207♦LBL 02
208 "CONVERGED SOLUT"
209 "⊢ION"
210 AVIEW
211 ADV
212 "V/F= "
213 ARCL 77
214 AVIEW
215 RCL 77
216 RCL 78
217 *
218 STO 80
219 "V="
220 ARCL X
221 AVIEW
222 RCL 78
223 X<>Y
224 -
225 STO 79
226 "L="
227 ARCL X
228 AVIEW
229 RCL 80
230 RCL 79
231 /
232 STO 79
233 "V/L="
234 ARCL X
235 AVIEW
236 ADV
237 "DETAILS ?,R/S"
238 PROMPT
239 XEQ 15
```

Table II

```
240 SCI 4
241 "    "
242 ASTO 83
243 "  "
244 ASTO 86
245 ARCL 83
246 "⊢ FLOWS"
247 PRA
248 CLA
249 XEQ 18
250 XEQ 15
```

Details output

```
251◆LBL 04
252 SF 07
253 SF 08
254 XEQ 16
255 FRC
256 RCL 78
257 *
258 STO 80
259 XEQ 08
260 /
261 "  "
262 ARCL X
263 ARCL 86
264 CF 07
265 RCL 80
266 XEQ 08
267 /
268 ARCL X
269 PRA
270 ISG 81
271 GTO 04
272 ADV
273 XEQ 15
274 CLA
275 ARCL 83
276 "⊢  "
277 "⊢MOL FRAC"
278 PRA
279 CLA
280 XEQ 18
281 FIX 5
282◆LBL 20
283 CLA
284 XEQ 16
285 FRC
286 STO 80
287 SF 07
288 XEQ 08
289 /
290 CF 08
291 XEQ 08
292 *
293 ARCL 86
294 ARCL X
295 ARCL 86
296 "⊢ "
297 CF 07
298 XEQ 08
299 RCL 80
300 *
301 SF 08
302 XEQ 08
303 /
304 ARCL X
305 PRA
306 ISG 81
307 GTO 20
308 RTN
309◆LBL 08
310 FS? 08
311 XEQ 14
312 FC? 07
313 1/X
314 RCL 79
315 FC? 07
316 1/X
317 FS? 08
318 *
319 1
320 +
321 RTN
322◆LBL 18
323 ARCL 86
324 "⊢LIQUID"
325 ARCL 83
326 "⊢VAPOR"
327 PRA
328 RTN
```

Calculates convergence function

```
329◆LBL 13
330 XEQ 16
331 FRC
332 XEQ 14
333 R↑
334 CLX
335 RDN
336 XEQ c
337 1
338 RCL 83
339 -
340 *
341 +
342 ISG 81
343 GTO 13
344 RTN
345◆LBL c
346 STO 83
347 1
348 -
349 RCL 77
350 *
351 1
352 +
353 /
354 RTN
```

K-value prediction subroutine

```
355◆LBL "KVAL"
356 RCL 84
357 XEQ 16
358 /
359 STO 79
360 1
361 X<=Y?
362 SF 00
363 RCL 85
364 RCL 81
365 100
366 +
367 RCL IND X
368 X<>Y
369 RDN
370 INT
371 /
372 STO 80
373 FS?C 00
374 GTO 01
375 2.415
376 ENTER↑
377 .7116
378 RCL 79
379 1/X
380 *
381 -
382 1.179
383 RCL 79
384 -2
385 Y↑X
386 *
387 -
388 .7072
389 RCL 79
390 -3
391 Y↑X
392 *
393 -
394 .1824
395 RCL 79
396 -4
397 Y↑X
398 *
399 +
400 XEQ J
401 *
402 GTO 02
403◆LBL 01
404 5.179
405 ENTER↑
406 5.133
407 RCL 79
408 1/X
409 *
410 -
411 .04566
412 RCL 79
413 -2
414 Y↑X
415 *
416 -
417 XEQ J
418 *
419◆LBL 02
420 1
421 RCL 79
422 1/X
423 -
424 5.366
425 *
426 +
427 E↑X
428 RCL 80
429 /
430 1
431 X<=Y?
432 SF 01
433 RDN
434 LN
435 STO 76
436 RCL 80
437 1
438 X>Y?
439 GTO 09
440 RDN
441 10
442 X>Y?
443 SF 03
444 X<=Y?
445 SF 04
446 GTO 10
447◆LBL 09
448 SF 02
```

Selects appropriate set of constants

```
449◆LBL 10
450 FS? 01
451 GTO 11
452 FS?C 02
453 1.014
454 FS?C 03
455 15.028
456 FS?C 04
457 29.042
458 GTO 12
459◆LBL 11
460 FS?C 02
461 43.053
462 FS?C 03
463 54.064
464 FS?C 04
465 65.075
466◆LBL 12
467 STO 82
468 RCL 80
469 LN
470 STO 80
471 FS?C 01
472 GTO 07
```

Calculates K_i for $K_R < 1.0$

```
473◆LBL 21
474 RCL IND 82
475 ISG 82
476 RCL IND 82
477 RCL 80
478 *
479 +
480 RCL 80
481 X↑2
482 ISG 82
483 RCL IND 82
484 *
485 +
486 RCL 80
487 3
488 Y↑X
489 ISG 82
490 RCL IND 82
491 *
492 +
493 ISG 82
494 STO IND 82
495 ISG 82
496 GTO 21
497 RCL 76
498 *
499 1
500 +
501 RCL 76
502 2
503 /
504 E↑X
505 *
506 1
507 -
508 RCL 82
509 6
510 -
511 RCL IND X
512 X<>Y
513 RDN
514 *
515 RCL 76
516 RCL 82
517 11
518 -
519 RCL IND X
520 X<>Y
521 RDN
522 *
523 +
524 E↑X
525 RTN
```

Calculates K_i for $K_R > 1.0$

```
526◆LBL 07
527 RCL IND 82
528 ISG 82
529 RCL IND 82
530 RCL 80
531 *
532 +
533 RCL 80
534 X↑2
535 ISG 82
```

(Continues next page)

Program performs vapor-liquid equilibrium calculations for the HP-41C calculator **Table II (cont'd)**

```
536 RCL IND 82
537 *
538 +
539 ISG 82
540 STO IND 82
541 ISG 82
542 GTO 07
543 RCL 76
544 3
545 Y↑X
546 *
547 RCL 76
548 X↑2
549 RCL 82
550 5
551 -
552 RCL IND X
553 X<>Y
554 RDN
555 *
556 +
557 RCL 76
558 RCL 82
559 9
560 -
561 RCL IND X
562 X<>Y
563 RDN
564 *
565 +
566 E↑X
567 RTN
```

Subroutine resets counter

```
568♦LBL 15
569 RCL 00
570 1000
571 /
572 1
573 +
574 STO 81
575 RTN
```

Retrieves ω

```
576♦LBL J
577 RCL 81
578 100
579 +
580 RCL IND X
581 X<>Y
582 RDN
583 FRC
584 RTN
```

Sets flag for BP calculation

```
585♦LBL B
586 SF 06
587 CF 05
588 GTO e
```

Sets flag for DP calculation

```
589♦LBL D
590 CF 06
591 SF 05
592♦LBL e
593 0
594 STO 89
595 FS? 05
596 RCL 90
597 FS? 06
598 RCL 88
599 1
600 X>Y?
601 SF 03
602 RCL 84
603 STO 83
604 100
605 FS?C 03
606 CHS
607 FS? 05
608 +
609 FS? 06
610 -
611 STO 84
612 RCL Z
613 LN
614 STO 87
615 XEQ 15
```

BP or DP interpolation

```
616♦LBL 19
617 XEQ "KVAL"
618 XEQ 16
619 FRC
620 X<>Y
621 FS? 05
622 /
623 FS? 06
624 *
625 ST+ 89
626 ISG 81
627 GTO 19
628 RCL 89
629 LN
630 RCL 87
631 X<>Y
632 -
633 RCL 87
634 X<>Y
635 /
636 RCL 84
637 1/X
638 RCL 83
639 1/X
640 -
641 *
642 RCL 83
643 1/X
644 +
645 1/X
646 459.67
647 -
648 FS?C 05
649 "DP="
650 FS?C 06
651 "BP="
652 ARCL X
653 "├ F"
654 RCL 83
655 STO 84
656 TONE 5
657 AVIEW
658 RTN
```

Subroutine retrieves z_i

```
659♦LBL 16
660 RCL 81
661 90
662 +
663 RCL IND X
664 X<>Y
665 RDN
666 RTN
```

Subroutine retrieves K_i

```
667♦LBL 14
668 RCL 81
669 110
670 +
671 RCL IND X
672 X<>Y
673 RDN
674 RTN
675 .END.
```

(Continued from p. 220)

$$X = \ln K_R = \ln\left(\frac{p_{ri}^0}{P_r}\right) \tag{16}$$

$$Z = \ln P_r \tag{17}$$

The values of the 21 regression coefficients (a_0–a_{20}) are given in Table I for three ranges of reduced pressure.

To evaluate K_R, a correlation of the reduced vapor pressure developed by Pitzer et al. [6] was used. This vapor pressure relationship is:

$$\ln p_r^0 = (\ln p_r^0)^0 + \omega\left(\frac{\partial \ln p_r^0}{\partial \omega}\right)_T \tag{18}$$

where $$(\ln p_r^0)^0 = 5.366(1 - T_r^{-1}) \tag{19}$$

For $T_r < 1.0$:

$$\left(\frac{\partial \ln p_r^0}{\partial \omega}\right)_T = 2.415 - 0.7116(T_r^{-1}) - 1.179(T_r^{-2}) - 0.7072(T_r^{-3}) + 0.1824(T_r^{-4}) \tag{20}$$

For $T_r > 1.0$:

$$\left(\frac{\partial \ln p_r^0}{\partial \omega}\right)_T = 5.179 - 5.133(T_r^{-1}) - 0.04566(T_r^{-2}) \tag{21}$$

Calculator program

The program was written using the algorithms described in Fig. 2, 3 and 4. If run on an HP-41C, a quad memory module is needed. The program listing is presented in Table II. The initial phase of the program is described in Fig. 2. After the total moles and number of components are entered, a loop is begun that inserts the component properties needed by "KVAL" (the subroutine that predicts the K-values) and also computes z_i (the component mole fraction in the feed).

After the pure-component properties are entered, the system temperature and pressure are punched in. These and all previous inputs are called up in the display, using the calculator's alphanumeric capacity. This prevents losing track of input status during interruptions. Next, the K_is are calculated via KVAL. As each K_i is calculated, it is displayed, and the corresponding z_i is added to the $(V/F)_1$ register if the K_i is greater than 1.0. This will provide the initial guess for the flash calculation. Following the K-value predictions, a check is made on the phase of the system. The following equations are used for this purpose:

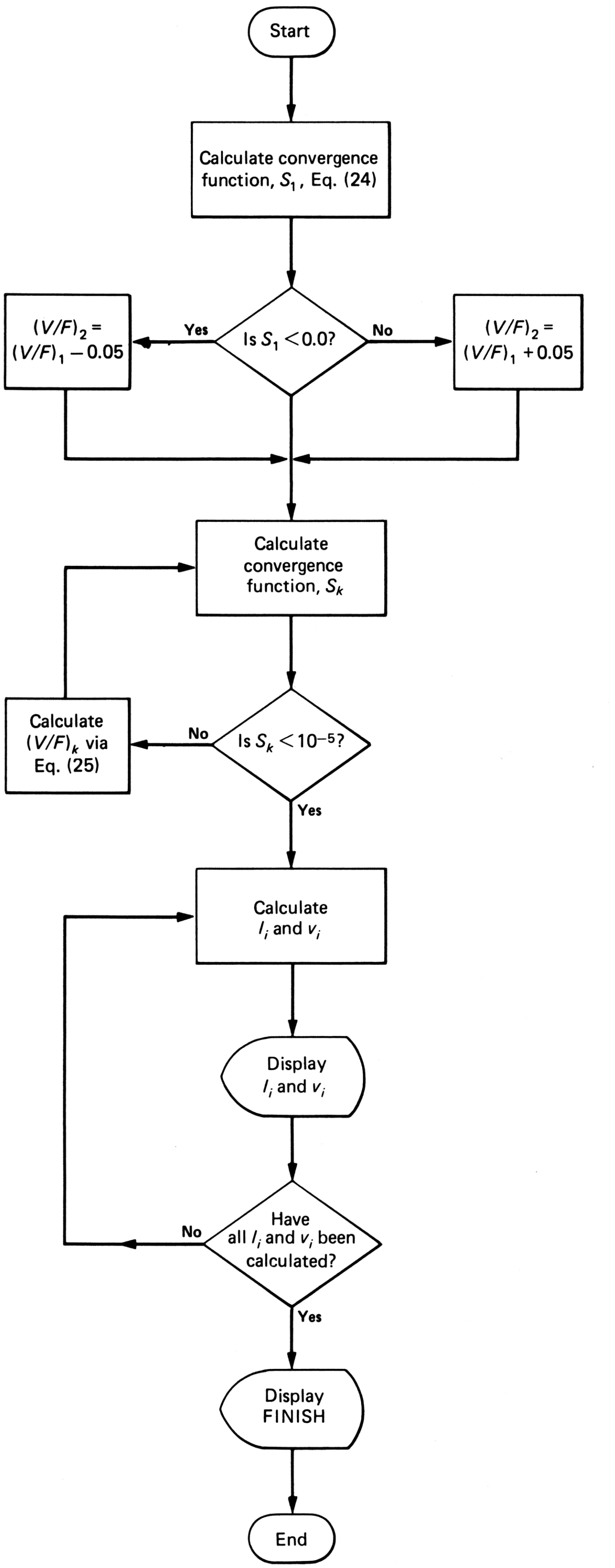
$$\Sigma z_i/K_i < 1.0 \text{ (the system is all vapor)} \tag{22}$$

$$\Sigma z_i K_i < 1.0 \text{ (the system is all liquid)} \tag{23}$$

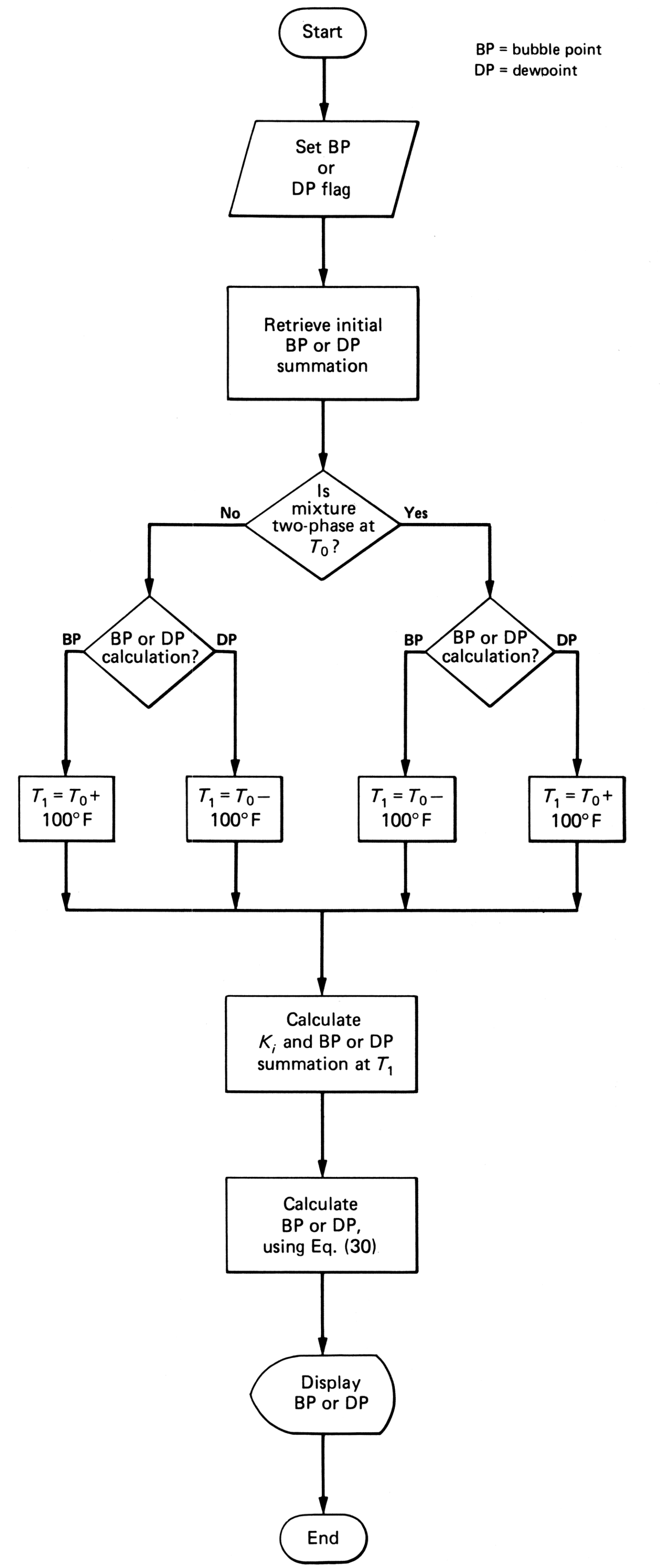
These checks result in a display indicating the phase of the system. This will prevent a flash calculation from being performed on a one-phase system. A computation of this type would not converge, or would converge to a meaningless result.

Fig. 3 describes the equilibrium flash algorithm used. This is a trial-and-error calculation on (V/F). A Newtonian convergence technique is used on the following function [7]:

$$S_k = \Sigma \frac{z_i(1 - K_i)}{(V/F)_k(K_i - 1) + 1} \tag{24}$$



This is the method the program uses to perform equilibrium flash calculations **Fig. 3**



Dewpoints and bubble points are found and then displayed by the program **Fig. 4**

User's instructions for running the program — Table III

Step	Instructions	Input	Function	DISPLAY
1.	Load program			
2.	Set size and load data		XEQ SIZE 121	
3.	Set user mode			
4.	Start		XEQ VLE	TOTAL MOLES = ?
5.	Enter moles		R/S	N = ?
6.	Enter no. of components		R/S	T_C UNITS = ?
7.	Enter units to be used for T_c	°F or R	R/S	T_{C1} = ? ⋮
8.	Enter component properties as asked for:			T = ?, DEG F
9.	Enter system temperature	°F	R/S	P = ?
10.	Enter system pressure Component K-values displayed	psia	R/S	K_1 = ⋮ K_n =
	System phase displayed			ABOVE DP BELOW BP TWO-PHASE
11.	At this point, one of four options exists:			
	I. Bubble point		B	BP =
	II. Dewpoint		D	DP =
	III. Flash—for detailed product information, press R/S. This will yield component flows and mole fractions for V and L.		C	S_k = ⋮ CONVERGED V/F = V = L = V/L = DETAILS ? R/S
	IV. Change T and P		E	

Storage register setup, use of flags, and assignments of the calculator's keys — Table IV

Data registers

Register	Contents
00	No. of components
01 ↓ 75	Regression coefficients
76	$(V/F)_k$, $\ln P_r$
77	$(V/F)_{k+1}$, K_R
78	Total moles
79	S_k, T_r
80	S_{k+1}, P_r
81	Counter
82	Counter
83	K_i
84	T
85	P
86	
87	$\ln(\Sigma^*)_1$
88	$\Sigma(z_iK_i)$
89	$(\Sigma^*)_2$
90	$(\Sigma z_i/K_i)_1$
91 ↓ 100	$T_{ci}z_i$
101 ↓ 110	$P_{ci}\omega_i$
111 ↓ 120	K_i

* either: z_iK_i or z_i/K_i

Flags

#	Init S/C	Set indicates
00	C	$T_r > 1.0$
01	C	$K_R > 1.0$
02	C	$P_r > 1.0$
03	C	$1.0 < P_r < 10.0$
04	C	$P_r > 10.0$
05	C	DP calculation
06	C	BP calculation
10	C	one-phase system

Assignments

Function	Key
VLE	A
BP	B
Flash	C
DP	D
Change	E

VLE = vapor-liquid equilibrium

S = set

C = clear

Register configuration for data cards — Table V

R00= 0.000000000	R16= -0.110103620	R32= 0.036108945	R48= 0.035372461	R64= 0.001369845
R01= 0.723546880	R17= -0.009820518	R33= 1.000000000	R49= 0.006731340	R65= 0.398601200
R02= -0.119552620	R18= 0.000851396	R34= -1.469887300	R50= -0.046076005	R66= -0.193352400
R03= -0.019175521	R19= 1.000000000	R35= 1.537564500	R51= -0.000602082	R67= 0.023885130
R04= -0.000790434	R20= -0.031743583	R36= -0.719064210	R52= -0.002218345	R68= 1.000000000
R05= 0.936718767	R21= -0.077912651	R37= 0.089098628	R53= -0.000478355	R69= 0.174301880
R06= -0.092938874	R22= -0.012739586	R38= 1.000000000	R54= 0.563198000	R70= -0.082957315
R07= -0.089253134	R23= -0.035998746	R39= -0.339242840	R55= -0.207628980	R71= 0.010571085
R08= -0.021210992	R24= 1.000000000	R40= 1.380265400	R56= -0.001581164	R72= 1.000000000
R09= -0.001102325	R25= 3.471993500	R41= -0.647461420	R57= 1.000000000	R73= -0.032969708
R10= 0.010910644	R26= -2.412893100	R42= 0.074000484	R58= -0.000190156	R74= 0.021278044
R11= 0.834858140	R27= 0.745485830	R43= 0.558239120	R59= 0.023954299	R75= -0.003227667
R12= -1.751046300	R28= -0.137130690	R44= -0.224173390	R60= -0.003804810	R76= 0.000000000
R13= -1.788251600	R29= 0.933225460	R45= -0.026665354	R61= 1.000000000	
R14= -0.202551450	R30= -0.298381490	R46= 1.015808088	R62= -0.001730038	
R15= 0.716139740	R31= 0.036108945	R47= -0.004611621	R63= -0.002241499	

With this function, convergence to 10^{-5} is usually attained in four to five trials. New guesses for $(V/F)_k$ are calculated by:

$$(V/F)_{k+1} = (V/F)_k - \left[\frac{(V/F)_k - (V/F)_{k-1}}{S_k - S_{k-1}}\right] S_k \quad (25)$$

As described earlier, $(V/F)_1$ was obtained assuming that all components with $K_i > 1.0$ were totally vapor. Fig. 3 describes how $(V/F)_2$ is determined. S_k is displayed after each trial, which allows for monitoring of the convergence. After convergence is attained, the l_i and v_i values are calculated and will be displayed.

Fig. 4 describes the bubble-point and dewpoint calculations. The algorithm used for the calculation is a simplified technique that eliminates the usual trial-and-error procedure. The conventional calculation would use the following equations in order to determine the dewpoint and bubble point:

$$f(T) = \Sigma z_i/K_i - 1.0 = 0.0 \text{ (dewpoint)} \quad (26)$$

$$f(T) = \Sigma z_i K_i - 1.0 = 0.0 \text{ (bubble point)} \quad (27)$$

A temperature would be guessed, and K-values deter-

Output of the printer for the example **Table VI**

Input*

```
VAPOR-LIQUID EQUILIBRIUM

TOT MOLES=?
        21,350.     RUN
N=?
            6.      RUN
TC UNITS=?
R                   RUN
TC1=?
        1,012.7     RUN
F1=?
        4,500.      RUN
PC1=?
        714.22      RUN
OMEGA1=?
          .215      RUN
TC2=?
        1,069.2     RUN
F2=?
        9,100.      RUN
```

```
PC2=?
        590.04      RUN
OMEGA2=?
         .2518      RUN
TC3=?
        1,138.      RUN
F3=?
        3,200.      RUN
PC3=?
        529.94      RUN
OMEGA3=?
         .2979      RUN
TC4=?
       1,114.6      RUN
F4=?
        1,900.      RUN
PC4=?
        509.95      RUN
OMEGA4=?
         .3164      RUN
```

```
TC5=?
        1,112.8     RUN
F5=?
        2,000.      RUN
PC5=?
        499.96      RUN
OMEGA5=?
         .3068      RUN
TC6=?
       1,136.07     RUN
F6=?
          650.      RUN
PC6=?
         465.4      RUN
OMEGA6=?
          .335      RUN
```

*The input "echo" will be surpressed if printed in manual mode.

Output

```
**
T=?, DEG F
        250.000     RUN
P=?
         18.000     RUN
                    RUN
K1=2.4008
K2=1.0677
K3=0.4449
K4=0.5081
K5=0.5238
K6=0.3596
*TWO PHASE*
                  XEQ C
S=0.1253
S=0.0060
S=-0.0001
S=2.7678E-7
CONVERGED SOLUTION
```

```
V/F= 0.3205
V=6,842.9320
L=14,507.0680
V/L=0.4717

DETAILS ?,R/S
                         RUN
            FLOWS
     LIQUID       VAPOR
     2.1103E3     2.3897E3
     6.0597E3     3.0403E3
     2.6449E3     5.5505E2
     1.5327E3     3.6733E2
     1.6038E3     3.9622E2
     5.5574E2     9.4256E1
```

```
        MOL FRAC
    LIQUID      VAPOR
    0.14546     0.34923
    0.41770     0.44430
    0.18232     0.08111
    0.10565     0.05368
    0.11055     0.05790
    0.03831     0.01377
                        XEQ B
BP=241.22502 F
                        XEQ D
DP=266.27314 F
```

```
XEQ E

**
T=?, DEG F
        280.00000     RUN
P=?
         18.00000     RUN
K1=3.4442
K2=1.6247
K3=0.6916
K4=0.7845
K5=0.8042
K6=0.5674
**ABOVE DP**
```

Notice that this new case is above the dewpoint.

mined at each temperature until the above functions equaled 0, within a given tolerance. A Newtonian convergence technique could be used to accelerate the convergence. However, a faster method is used here by making modifications to Eq. (26) or (27) to yield a more nearly linear function on which to apply the convergence technique. Since K_i is related to vapor pressure (see Eq. (6)), one improvement would be:

$$g(T) = \ln \Sigma z_i/K_i(\text{or } z_iK_i) = 0.0 \qquad (28)$$

Since the vapor pressure is related to T^{-1}, a further improvement would be:

$$g(T^{-1}) = \ln \Sigma z_i/K_i(\text{or } z_iK_i) = 0.0 \qquad (29)$$

In most cases encountered with the program, Eq. (29) results in a plot that is very nearly a straight line. Thus, the bubble point or dewpoint can be obtained from a linear interpolation of Eq. (29) between T_0 and T_1. Here, T_0 is the program's first guess for T, and T_1 is its second guess.

$$\frac{1}{T_{bp}}\left(\text{or } \frac{1}{T_{dp}}\right) = \frac{1}{T_0} + \left(\frac{1}{T_1} - \frac{1}{T_0}\right)\frac{g(1/T_0)}{g(1/T_0) - g(1/T_1)} \qquad (30)$$

Fig. 4 describes how T_1 is obtained.

Table III lists the instructions for using the program. Table IV describes the storage register setup, use of flags, and assignment of the calculator's keys.

To produce the data cards required for this program, the register contents should be set up as shown in Table V. Then, the WDTA function can be used to produce the data cards.

Example

The feed to the benzene tower of an aromatics extraction unit is as follows:

	lb-mol/h
Benzene	4,500
Toluene	9,100
o-xylene	3,200
m-xylene	1,900
p-xylene	2,000
i-propylbenzene	650
	21,350

The feed is at 18 psia and 250°F. Determine the vapor-liquid split and the equilibrium compositions. Also, determine the bubble point and dewpoint to help set the feed-preheater operating limits.

The ideal-vapor-solution assumption should be valid (i.e., $P < 20$ atm). Also, the ideal-liquid-solution assumption should be valid, since it applies to a system of reasonably-close-boiling homologs at pressures below 10 atm. This system could be considered a borderline case for the ideal-liquid-solution assumption, and should give some indication of the accuracy of this program near the limit of its applicability.

First, the input data must be obtained. The best data to use with this program are the pure-component properties contained in Edmister's book [*1*]. Since these data were used in developing the K-value correlation, they will yield the most accurate results. For components not included in Edmister's compilation, any other available source can be used. An excellent one is Reid, et al. [*8*].

Results

Following the input procedure outlined in Fig. 2, these results were obtained, and are compared with those determined by using the Soave-Redlich-Kwong (SRK) method on a process simulator:

	Liquid		Vapor	
	HP-41C	SRK	HP-41C	SRK
Benzene	2,110	2,151	2,390	2,349
Toluene	6,060	6,079	3,040	3,021
o-xylene	2,645	2,673	555	527
m-xylene	1,533	1,547	367	353
p-xylene	1,604	1,620	396	380
i-propylbenzene	556	560	94	91
	14,508	14,630	6,842	6,721

SRK: $T_{bp} = 241$°F, $T_{dp} = 266$°F
HP-41C: $T_{bp} = 240$°F, $T_{dp} = 265$°F

With no modifications, this program can be used with the HP-41C printer. The results generated are shown in Table VI. This printout includes verification of the inputs, plus the values generated by the program.

The SRK equation-of-state provided predictions of the liquid volumetric properties needed to calculate ϕ_i^L and γ_i^L. Thus, the SRK computer simulation assumed neither ideal-vapor nor ideal-liquid solutions. As can be seen, the difference between these two methods is negligible for the dew-point and bubble-point calculations, and small for the flash calculation.

Program comments

1. The register configuration as shown in Table V is correct. Some confusion has arisen from the fact that although registers 1–75 are given values, only 63 constants are listed in Table I. This discrepancy is due to the fact that interspersed among these 75 registers are 12 "scratch" registers (5, 10, 19, 24, 33, 38, 46, 50, 57, 61, 68, 72). The content of these registers will not affect the program results.
2. A common mistake involving program lines 39 and 56 should be mentioned. These lines execute the "round" function designated by **RND,** not the more often used "roll down" function designated by **RDN.**
3. Due to storage limitations of the TI calculators, there is no TI version of this program.

References

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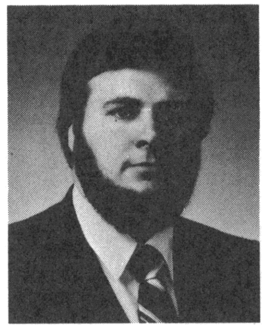

The author

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Evaluating separation processes

This calculator program uses stream-composition data to determine the best-fit mass balance for a working separator.

Raymond M. Ingels, California Air Resources Board

☐ Mass balances for separation processes are easily calculated from measurements of flowrate and stream composition. But such balances usually do not close—i.e., do not account for 100% of each component—because of errors in flow measurement and chemical analysis.

This program, written for the HP-97 programmable calculator, closes the overall mass balance perfectly. It also determines the best-fit (i.e., least-squared-error) mass balance for each component, up to a maximum of eight.

The method of the program applies to any separation process, but the program itself applies specifically to separation units that split one feedstream into two streams—e.g., distillation columns, absorbers, scrubbers, adsorption units. The program uses only composition data, which tend to be more accurate than flow data.

The key result is an accurate estimate of the fraction of each component leaving in each of the two streams. This can be a measure of separation efficiency. The results may also be used to check the consistency of flowrate and chemical-composition measurements.

The one-component case

Anderson [1] showed how to use chemical composition data to calculate the split of a single component between two discharge streams. For a generalized separator, as in the figure, the overall and component mass balances are:

$$F = E + R \quad (1)$$

$$Fx_f = Ex_e + Rx_r \quad (2)$$

where F, E and R are the mass flowrates of the feed and product streams, and x_f, x_e and x_r are the mass fractions of the component in those streams. Solving the two equations simultaneously yields Z_e, the fraction of the component that leaves in Stream E (extract or overhead):

$$Z_e = Ex_e/Fx_f = x_e(x_f - x_r)/(x_e - x_r)x_f \quad (3)$$

Eq. 3 closes both the overall mass balance (Eq. 1) and the component one (Eq. 2) perfectly, despite experimental error, because it uses only one set of compositions.

How the program works

Because of experimental error in the chemical analyses, it is impossible to get the overall and component mass balances to close perfectly when there are several components. That is, Eq. 1 and Eq. 2 will yield a different estimate of the split (E/F and R/F) for each set of component data.

Finding the best estimate of the split requires a least-squared-error analysis. In the program, the analysis is an extension of that in [2]. The sum of the squared errors in the component mass balances is minimized, subject to the constraint that the overall mass balance closes perfectly:

The overall mass balance is:

$$W_e + W_r = E/F + R/F = 1 \quad (4)$$

where W_e and W_r are the mass fractions of the feedstream leaving in Streams E and R, respectively. The mass balance for each of the n components is:

$$Z_{ei} + Z_{ri} = 1 \quad (5)$$

where:

$Z_{ei} = (x_{ei}/x_{fi})W_e$
= Fraction of component i leaving in Stream E

$Z_{ri} = (x_{ri}/x_{fi})W_r$
= Fraction of component i leaving in Stream R

If we let $a_i = (x_{ei}/x_{fi})$, and $b_i = (x_{ri}/x_{fi})$, then the component mass balance for component i may be rewritten as:

$$a_i\, W_e + b_i\, W_r = 1 \quad (6)$$

Since a_i and b_i are based on chemical analyses, the Eq. 6 balances will not close perfectly. In other words, there will be a residual, v_i, for each mass balance:

$$v_i = a_i\, W_e + b_i\, W_r - 1 \quad (7)$$

Now, the objective is to minimize the sum of the squared residuals for the n components. Formally: Minimize $f = (v_1^2 + v_2^2 + \dots v_n^2)$, subject to the constraint that $\Psi = W_e + W_r - 1 = 0$.

The Lagrangian multiplier procedure for minimizing a function subject to an equality constraint [3] requires simultaneous solution of the following equations:

$$\frac{\delta f}{\delta W_e} + \lambda \frac{\delta \Psi}{\delta W_e} = 0 \quad (8)$$

$$\frac{\delta f}{\delta W_r} + \lambda \frac{\delta \Psi}{\delta W_r} = 0 \quad (9)$$

$$W_e + W_r - 1 = 0 \quad (10)$$

Originally published May 30, 1983.

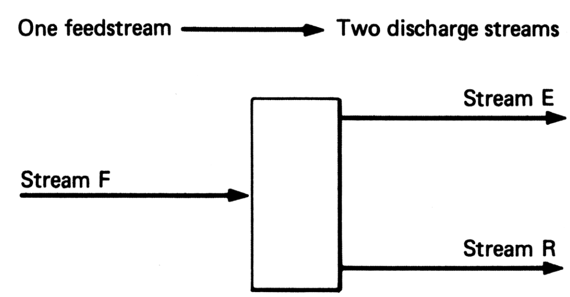
Program listing for HP-97 calculator (can be modified for HP-67) **Table I**

Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	030	X≤Y?	16-35	059	RCL2	36 02
002	CLRG	16-53	031	GTO3	22 03	060	-	-45
003	P⇄S	16-51	032	1	01	061	÷	-24
004	CLRG	16-53	033	+	-55	062	STO0	35 00
005	P⇄S	16-51	034	STOI	35 46	063	CHS	-22
006	2	02	035	RCLi	36 45	064	ENT↑	-21
007	4	04	036	X²	53	065	1	01
008	STOI	35 46	037	ST+4	35-55 04	066	+	-55
009	1	01	038	RCLi	36 45	067	PRTX	-14
010	RTN	24	039	DSZI	16 25 46	068	STO1	35 01
011	*LBLB	21 12	040	RCLi	36 45	069	RCL0	36 00
012	R↓	-31	041	×	-35	070	PRTX	-14
013	X⇄Y	-41	042	ST+3	35-55 03	071	SPC	16-11
014	÷	-24	043	DSZI	16 25 46	072	SPC	16-11
015	STOi	35 45	044	RTN	24	073	SPC	16-11
016	ST+6	35-55 06	045	*LBLC	21 13	074	2	02
017	DSZI	16 25 46	046	RCL3	36 03	075	4	04
018	LSTX	16-63	047	RCL4	36 04	076	STOI	35 46
019	R↑	16-31	048	-	-45	077	*LBL1	21 01
020	X⇄Y	-41	049	RCL5	36 05	078	CLX	-51
021	÷	-24	050	-	-45	079	ENT↑	-21
022	STOi	35 45	051	RCL6	36 06	080	RCLi	36 45
023	ST+5	35-55 05	052	+	-55	081	X=Y?	16-33
024	X²	53	053	2	02	082	GTO2	22 02
025	ST+2	35-55 02	054	ENT↑	-21	083	RCL1	36 01
026	RCLI	36 46	055	RCL3	36 03	084	×	-35
027	ENT↑	-21	056	×	-35	085	PRTX	-14
028	7	07	057	RCL4	36 04	086	DSZI	16 25 46
029	X⇄Y	-41	058	-	-45	087	RCLi	36 45

User instructions **Table II**

Step/description	Enter	Press	Display	Printout
1. Initialize registers		[A]	1.0000	
2. Enter Component 1 data	$x_{f1}\uparrow\ x_{e1}\uparrow\ x_{r1}$	[B]		
3. Repeat Step 2 for Components 2–n	$x_{fi}\uparrow\ x_{ei}\uparrow\ x_{ri}$	[B]		
4. Calculate results		[C]		E/F
				R/F
Component 1 results				Z_{e1}
				Z_{r1}
				$(Z_{e1}+Z_{r1})$
Components 2–n results				Z_{e2}, etc.

Note: Limit is eight components. If more are entered, the program will produce an overflow display.



Program applies to such separation processes

where λ is a multiplier whose numerical value is of no particular interest.

Performing the differentiations, and collecting terms, we obtain the three equations that the program has to solve simultaneously:

$$2\,W_e\Sigma a_i^2 + 2\,W_r\,\Sigma a_i\,b_i - 2\Sigma a_i + \lambda = 0 \quad (11)$$

$$2\,W_e\Sigma a_i\,b_i + 2\,W_r\Sigma b_i^2 - 2\Sigma b_i + \lambda = 0 \quad (12)$$

$$W_e + W_r - 1 = 0 \quad (13)$$

The program solves these equations, yielding values of W_e and W_r (E/F and R/F), and calculates Z_{ei} and Z_{ri} for each component. The Z values describe the performance of the separation unit; the E/F and R/F values can be compared with those calculated from flowmeter data to show whether the flow data are consistent with the chemical analyses. The program also sums the Z_{ei} and Z_{ri} values, indicating the degree of closure for each component—a sum of 1 is perfect, but the typical sum will be higher or lower than 1.

(Continued) Table I

Step	Key	Code
088	RCL0	36 00
089	x	-35
090	PRTX	-14
091	+	-55
092	PRTX	-14
093	SPC	16-11
094	DSZI	16 25 46
095	GT01	22 01
096	*LBL2	21 02
097	R/S	51
098	*LBL3	21 03
099	CLX	-51
100	1/X	52
101	R/S	51

Note: To modify the program for the HP-67 calculator: Substitute "R/S" for "PRTX" at locations 067, 070, 085, 090 and 092; and delete "SPC" at locations 071, 072, 073 and 093.

How to use the program

Table I is the program listing for the HP-97 calculator. To use the program on an HP-67, make the modifications listed in the notes. Table II lists instructions for using the program.

The program applies only to processes that take one feedstream and split it into two streams, and it has a limit of eight components. If more are entered, an error message will result.

Example

Table III lists chemical-analysis data for four components in each of the three streams in a separation unit. If we calculated *E/F* or *R/F* based on these data, we would have four different estimates.

Using the program, we first initialize the registers, then enter the data in order—x_f, x_e, x_r—for each component. Once all the data are entered, the program calculates *E/F* and *R/F*, plus Z_e, Z_r and ($Z_e + Z_r$) for each of the four decimal places by the calculator, for the example. Note that *E/F* (0.3112) and *R/F* (0.6888) add up to 1, so the overall mass balance closes.

Interpreting the results

The program's primary results are the recoveries of the components; that is, the fraction of each component leaving in each stream. These may be used to calculate the separation efficiency.

A byproduct result is the closure data. By sampling, analyzing and calculating closure a number of times, it is possible to determine whether the closure errors are random (i.e., the measurements are consistent) and whether there are calibration errors in the instruments that analyze composition. (The statistics are beyond the scope of this article.) Likewise, comparing the program's *E/F* and *R/F* result with that calculated from flowmeter data can identify inconsistencies in the flowmeters.

Example data and results **Table III**

Data:

	Mass fraction in stream		
Component	F	E	R
1	0.2125	0.2043	0.2154
2	0.2926	0.1243	0.4047
3	0.1124	0.2452	0.0517
4	0.1724	0.2903	0.1456

Results:

E/F (overall fraction in Stream E)	0.3112	***
R/F (overall fraction in Stream R)	0.6888	***
Z_{e1} (fraction in Stream E)	0.2992	***
Z_{r1} (fraction in Stream R)	0.6982	***
($Z_{e1} + Z_{r1}$) (= 1 if perfect closure)	0.9974	***
Z_{e2}	0.1322	***
Z_{r2}	0.9527	***
($Z_{e2} + Z_{r2}$)	1.0849	***
Z_{e3}	0.6788	***
Z_{r3}	0.3168	***
($Z_{e3} + Z_{r3}$)	0.9957	***
Z_{e4}	0.5240	***
Z_{r4}	0.5816	***
($Z_{e4} + Z_{r4}$)	1.1057	***

For TI users

The program for TI users is found in Table IV. User instructions are in Table V, and the example with a printout of the results is in Table VI. The TI version is run the same way as the HP version, and yields the results in the same order.

Program listing for TI version **Table IV**

Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	011	59	59	022	59	59
001	11	A	012	91	R/S	023	95	=
002	47	CMS	013	42	STO	024	72	ST*
003	02	2	014	58	58	025	00	00
004	04	4	015	91	R/S	026	44	SUM
005	42	STO	016	42	STO	027	06	06
006	00	00	017	57	57	028	01	1
007	91	R/S	018	43	RCL	029	22	INV
008	76	LBL	019	58	58	030	44	SUM
009	12	B	020	55	÷	031	00	00
010	42	STO	021	43	RCL	032	43	RCL

(Continued) Table IV

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
033	57	57	061	00	00	089	43	RCL	117	95	=	145	54	54
034	55	÷	062	33	X²	090	04	04	118	99	PRT	146	22	INV
035	43	RCL	063	44	SUM	091	75	-	119	42	STO	147	01	1
036	59	59	064	04	04	092	43	RCL	120	55	55	148	22	INV
037	95	=	065	73	RC*	093	05	05	121	43	RCL	149	44	SUM
038	72	ST*	066	00	00	094	85	+	122	56	56	150	00	00
039	00	00	067	32	X⇄T	095	43	RCL	123	99	PRT	151	73	RC*
040	44	SUM	068	01	1	096	06	06	124	98	ADV	152	00	00
041	05	05	069	22	INV	097	95	=	125	98	ADV	153	65	×
042	33	X²	070	44	SUM	098	55	÷	126	98	ADV	154	43	RCL
043	44	SUM	071	00	00	099	53	(	127	02	2	155	56	56
044	02	02	072	73	RC*	100	02	2	128	04	4	156	95	=
045	08	8	073	00	00	101	65	×	129	42	STO	157	99	PRT
046	32	X⇄T	074	65	×	102	43	RCL	130	00	00	158	85	+
047	43	RCL	075	32	X⇄T	103	03	03	131	76	LBL	159	43	RCL
048	00	00	076	95	=	104	75	-	132	23	LNX	160	54	54
049	77	GE	077	44	SUM	105	43	RCL	133	00	0	161	95	=
050	22	INV	078	03	03	106	04	04	134	32	X⇄T	162	99	PRT
051	55	÷	079	01	1	107	75	-	135	73	RC*	163	98	ADV
052	00	0	080	22	INV	108	43	RCL	136	00	00	164	01	1
053	95	=	081	44	SUM	109	02	02	137	67	EQ	165	22	INV
054	91	R/S	082	00	00	110	54	)	138	24	CE	166	44	SUM
055	76	LBL	083	91	R/S	111	95	=	139	65	×	167	00	00
056	22	INV	084	76	LBL	112	42	STO	140	43	RCL	168	61	GTO
057	01	1	085	13	C	113	56	56	141	55	55	169	23	LNX
058	44	SUM	086	43	RCL	114	94	+/-	142	95	=	170	76	LBL
059	00	00	087	03	03	115	85	+	143	99	PRT	171	24	CE
060	73	RC*	088	75	-	116	01	1	144	42	STO	172	91	R/S

User instructions for TI version **Table V**

Step/description	Enter	Press	Display	Print
1. Load program				
2. Clear registers and set counter for data		A	24.	
3. Enter data for each component	x_{f1}	B	x_{f1}	
	x_{e1}	R/S	x_{e1}	
	x_{r1}	R/S	1.	
4. Repeat step 3 for the remaining components, up to eight components				
5. Start calculations		C		
6. Program will calculate and print:				
			E/F	
			R/F	
			Z_{e1}	
			Z_{r1}	
			$(Z_{e1} + Z_{r1}$	
			Z_{e2}, etc.	

Example for TI version **Table VI**

Load program and Press **A** to clear registers and set the counter for data.

Data:

Component	Mass fraction in stream *F*		*E*		*R*	
1	0.2125	**B**	0.2043	**R/S**	0.2154	**R/S**
2	0.2926	**B**	0.1243	**R/S**	0.4047	**R/S**
3	0.1124	**B**	0.2452	**R/S**	0.0517	**R/S**
4	0.1724	**B**	0.2903	**R/S**	0.1456	**R/S**

Press **C**:

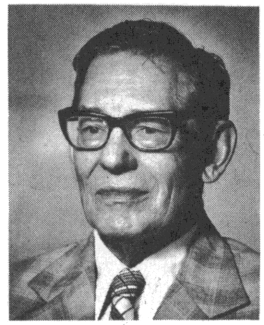
Results:

E/F (overall fraction in stream E)	.3111685208
R/F (overall fraction in stream R)	.6888314792
Z_{e1} (fraction in stream E)	.2991610767
Z_{r1} (fraction in stream R)	.6982320029
$(Z_{e1} + Z_{r1})$ (= 1 if perfect closure)	.9973930796
Z_{e2}	0.132108131
Z_{r2}	.9527344485
$(Z_{e2} + Z_{r2})$	1.08492258
Z_{e3}	.6788124671
Z_{r3}	.3168379669
$(Z_{e3} + Z_{r3})$	.9956504339
Z_{e4}	.5239680027
Z_{r4}	.5817509476
$(Z_{e4} + Z_{r4})$	1.10571975

References

1. Anderson, Mark C., Recovery calculation for a separation process, *Chem. Eng.*, Dec. 19, 1977.
2. Ingels, R. M., How to solve non-compatible simultaneous equations, *Chem. Eng.*, Oct. 26, 1964.
3. Sokolnikoff, I. S., and Redheffer, R. M., "Mathematics of Physics and Modern Engineering," McGraw-Hill, New York, 1958, pp. 249–257.

The author



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Optimizing reactor agitation in heat-transfer-limited situations

The optimum agitator design for a reactor can be determined from heat-transfer considerations. This program for the TI-59 performs the tedious calculations involved in evaluating heat-transfer and agitator-power-consumption relationships.

Michael E. Bowsher *and* ***David F. Hooley****, Mobay Chemical Corp.*

☐ The chemical engineer is often faced with trying to increase the productivity of existing or proposed reactor systems in which heat transfer is limiting in at least one of the processing steps. Reactor agitator design can have a significant effect on reactor productivity, but many times is not thoroughly investigated. The engineer can usually determine an agitator configuration that would yield a reasonably high level of productivity via improved heat transfer. However, constantly changing viscosities, multi-product reactor situations, and heating and/or cooling requirements must be taken into account, and all of these can grossly affect the configuration of the "best" agitator design. Because of time constraints, the engineer is seldom able to determine a truly optimum design for all variations.

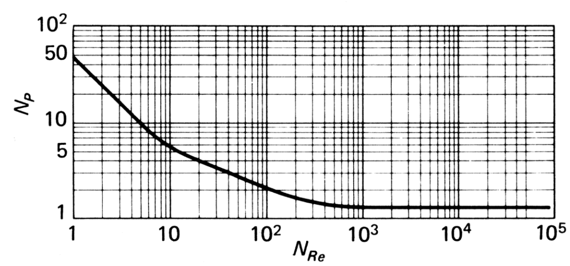
It is not uncommon to find that the agitator designs of recently installed reactor systems miss the optimum design point by as much as 30% or more. Considering the multimillion-dollar cost per unit for new sophisticated reactor installations, the resulting loss in productivity can have a major adverse effect on both production costs and total project capital costs.

[For a more complete treatment of mixing in vessels, including a section on heat transfer, see the report entitled "Fluid mixing technology and practice," that appeared in *CE*'s June 13 issue, beginning on p. 82. For additional information specifically on evaluating heat transfer in agitated vessels, see "Heat transfer in agitated vessels," beginning on p. 62 of the April 4, 1983, issue.—*Ed.*]

The agitator optimization study

The authors' need to expand production capabilities prompted an agitator optimization study to identify a way of reducing total capital costs by reducing the number of new reactor units to be installed. Agitator optimization to reduce cycle times was one of several alternatives evaluated.

The agitation study attempted to: (1) optimize agitator configuration to maximize heat transfer; (2) design a system capable of handling materials over a viscosity range of 1 to 50,000 cP; (3) utilize the lowest rotational speed possible to extend agitator seal life; and (4) minimize the required agitator motor size, and attempt to use a single-speed motor.



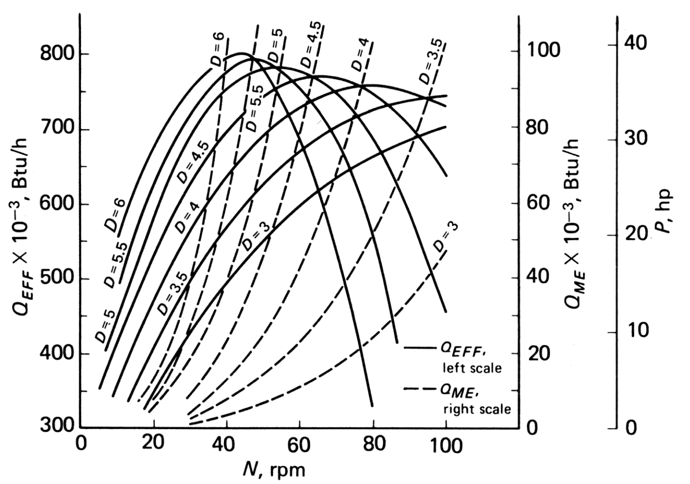
Power number as a function of Reynolds number for a 6-blade agitator **Fig. 1**

Large-diameter so-called "modified axial paddle" agitator blades were judged, based on the reference by Uhl and Gray, to be the best type of blade to efficiently handle materials in the viscosity range under consideration. General equations, which are included under "Calculated Terms" in the Nomenclature box, were developed for this type of blade to describe turbine power consumption (as shown in Fig. 1) and heat transfer.

The TI-59 calculator program presented in Table I was developed based on those equations. The results can be used to evaluate which configuration would be the optimum for the situation at hand. Once this has been determined, it is easy to generate additional data to evaluate the effects of:

- Changes in the density of the liquid on agitator horsepower requirements.
- Changes in the specific heat of the liquid on heat transfer.
- Cooling media temperature on the effective heat-transfer rate.
- Thermal conductivity on heat transfer.

Originally published June 27, 1983.



Heat transfer and power requirements vs. agitator speed for various impeller diameters **Fig. 2**

Using the program

The program listed in Table I, and the data, can be stored on four sides of magnetic cards. All ten data-input keys are used to place variable information into the data memory. Once a new set of input data is placed into memory, it may be retained for future calculations by rerecording card side 4, if that should be desired.

To perform the calculations, follow the input steps as outlined in Table II, "User instructions." The initial data—impeller diameter, impeller speed, density, viscosity (bulk and wall), heat capacity, thermal conductivity, etc.—are entered. The program calculates the effective heat-transfer rate, Q_{EFF}, the agitator power consumption, P, and the total heat transferred, Q_{HE}, at the chosen agitator speed. To calculate Q_{EFF} at various values of N, repeat Steps 3a-3i as required to modify the input data, and Step 4 to initiate the calculation. The results of such a set of single runs, for the example to be discussed later, are plotted as one of the solid lines in Fig. 2.

For a chain calculation, enter the initial and final agitator speeds, N_1 and N_2, and the number of trials, n. A new set of Q_{EFF} vs. N values is generated, which can be plotted. This continues until a family of curves at a given viscosity has been plotted, as shown by the series of solid lines in Fig. 2. This can be repeated for as many viscosities as needed.

Different agitation systems

The program results have been compared only with data on baffled agitation systems that employ pitched-blade turbines with D/T ratios of between 0.3 and 0.8, and with turbine spacings equal to or greater than D. Reynolds numbers were in the range of about 10 to 30,000.

However, this program may also be used to analyze quite different agitation systems, without major revisions to the program, by doing the following:

1. Run the program, and compare the calculated horsepower with that actually determined from motor amperage measurements. Remember that motor inefficiencies and gear-box and seal frictional losses have to be deducted so that only actual turbine-related horsepower quantities are compared.

2. If a significant difference is found, adjust β by:

$$\beta' = \beta[P_{(determined)}/P_{(calculated)}]$$

3. Rerun the program, substituting β' for β. Within reasonable limits, the power number and, hence, the calculated horsepower, should be corrected for the agitation system under consideration, and it should be possible to vary the other power-related parameters as well.

Realizing that dissimilar agitation systems can have markedly different heat-transfer characteristics, an involved programming modification may be avoidable by using the following approach.

4. First, adjust β, as outlined above. Run the program to calculate Q_{EFF}. Compare this value with a value for

Nomenclature

- A — Heat-transfer area, ft^2
- C_p — Specific heat, Btu/(lb)(°F)
- D — Agitator impeller dia., ft
- h_o — Outside film coefficient, Btu/(h)(ft^2)(°F)
- h_{do} — Outside fouling factor, Btu/(h)(ft^2)(°F)
- h_{di} — Inside fouling factor, Btu/(h)(ft^2)(°F)
- N — Agitator speed, rpm; N_1 = initial value for N to be used in chain calculation; N_2 = final value for N to be used in chain calculation
- n — Number of agitator speed trials to be used in chain calculation
- k — Thermal conductivity, Btu/(h)(ft)(°F)
- T — Vessel dia., ft
- Δt — Log mean temperature difference, °F
- β — Number of turbines
- ρ — Liquid density, lb/ft^3
- μ — Bulk-liquid viscosity, cP
- μ_w — Wall viscosity, cP

Calculated terms:

- h_i — Inside film coefficient, Btu/(h)(ft^2)(°F); $h_i = 0.44(k/T)N_{Re}^{0.667}N_{Pr}^{0.333}(\mu/\mu_w)^{0.24}$
- H_o — Coefficient for heat transfer (except for the inside film coefficient's contribution), Btu/(h)(ft^2)(°F); $H_o = 1/(1/h_o + 1/h_{di} + 1/h_{do})$
- N_P — Power number (for a 4-bladed impeller): $N_P = 0.97605$ for $N_{Re} > 600$; $= 0.723\exp(1.6907 - 0.21788\ln N_{Re})$ for $100 < N_{Re} < 600$; $= 0.723\exp(2.7373 - 0.4424\ln N_{Re})$ for $10 < N_{Re} < 100$
- N_{Pr} — Prandtl number; $N_{Pr} = 2.4C_p\mu/k$
- N_{Re} — Reynolds number; $N_{Re} = 24.8D^2N\rho/\mu$
- P — Agitator-shaft power consumption, hp; $P = Q_{ME}/2{,}550$
- Q_{EFF} — Effective heat removal, Btu/h; $Q_{EFF} = Q_{HE} - Q_{ME}$
- Q_{HE} — Heat transferred, Btu/h; $Q_{HE} = UA\Delta t$
- Q_{ME} — Mechanical heat of agitation, Btu/h; $Q_{ME} = 6.67 \times 10^{-7}\beta N_P D^5 N^3 \rho$
- U — Overall heat-transfer coefficient, Btu/(h)(ft^2)(°F); $U = 1/(1/h_i + 1/H_o)$

Program for TI-59 evaluates heat-transfer and power requirements for numerous reactor-agitator configurations Table I

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
(1) 000	76	LBL	062	01	1	124	03	3	186	04	04	248	03	03	310	93	.
001	11	A	063	00	0	125	03	3	187	43	RCL	249	02	2	311	04	4
002	42	STO	064	00	0	126	00	0	188	16	16	250	04	4	312	04	4
003	03	03	065	42	STO	127	00	0	189	69	OP	251	04	4	313	95	=
004	99	PRT	066	00	00	128	00	0	190	06	06	252	02	2	314	42	STO
005	91	R/S	067	43	RCL	129	69	OP	(16) 191	03	3	253	02	2	315	01	01
(2) 006	76	LBL	068	11	11	130	04	04	192	06	6	254	04	4	316	02	2
007	12	B	069	91	R/S	131	43	RCL	193	04	4	255	03	3	317	03	3
008	22	INV	(10) 070	42	STO	132	04	04	194	00	0	256	07	7	318	00	0
009	86	STF	071	00	00	133	69	OP	195	02	2	257	04	4	319	00	0
010	01	01	072	99	PRT	134	06	06	196	03	3	258	05	5	320	02	2
011	42	STO	073	91	R/S	135	65	×	197	03	3	259	69	OP	321	04	4
012	04	04	(11) 074	76	LBL	136	01	1	198	07	7	260	04	04	322	03	3
013	99	PRT	075	17	B'	137	06	6	199	69	OP	261	69	OP	323	01	1
014	01	1	076	42	STO	138	01	1	200	04	04	262	05	05	324	69	OP
015	42	STO	077	12	12	139	07	7	201	43	RCL	263	43	RCL	325	04	04
016	19	19	078	99	PRT	140	03	3	202	10	10	264	11	11	326	43	RCL
017	43	RCL	079	91	R/S	141	01	1	203	69	OP	265	99	PRT	327	01	01
018	04	04	(12) 080	76	LBL	142	03	3	204	06	06	266	95	=	328	69	OP
019	91	R/S	081	18	C'	143	06	6	205	65	×	(17) 267	45	Y^x	329	06	06
(3) 020	42	STO	082	42	STO	144	69	OP	206	43	RCL	268	93	.	(18) 330	35	1/X
021	17	17	083	13	13	145	04	04	207	08	08	269	03	3	331	85	+
022	99	PRT	084	99	PRT	146	43	RCL	208	65	×	270	03	3	332	69	OP
023	02	2	085	91	R/S	147	07	07	209	02	2	271	03	3	333	00	00
024	42	STO	(13) 086	76	LBL	148	69	OP	210	93	.	272	65	×	334	02	2
025	19	19	087	19	D'	149	06	06	211	04	4	273	53	(	335	03	3
026	43	RCL	088	42	STO	150	65	×	212	55	÷	274	43	RCL	336	00	0
027	17	17	089	14	14	151	02	2	213	03	3	275	09	09	337	00	0
028	91	R/S	090	99	PRT	152	04	4	214	07	7	276	55	÷	338	69	OP
(4) 029	42	STO	091	91	R/S	153	93	.	215	02	2	277	43	RCL	339	04	04
030	19	19	(14) 092	76	LBL	154	08	8	216	03	3	278	08	08	340	69	OP
031	99	PRT	093	10	E'	155	55	÷	217	01	1	279	54	)	341	05	05
032	91	R/S	094	42	STO	156	04	4	218	07	7	280	45	Y^x	342	00	0
(5) 033	76	LBL	095	15	15	157	02	2	219	03	3	281	93	.	343	01	1
034	13	C	(15) 096	99	PRT	158	02	2	220	05	5	282	02	2	344	69	OP
035	42	STO	097	98	ADV	159	04	4	221	03	3	283	04	4	345	04	04
036	07	07	098	98	ADV	160	03	3	222	00	0	284	94	+/-	346	43	RCL
037	99	PRT	099	76	LBL	161	06	6	223	69	OP	285	65	×	347	00	00
038	91	R/S	100	53	(	162	01	1	224	01	01	286	43	RCL	348	69	OP
(6) 039	76	LBL	101	22	INV	163	05	5	225	01	1	287	16	16	349	06	06
040	14	D	102	58	FIX	164	69	OP	226	03	3	288	45	Y^x	350	35	1/X
041	42	STO	103	22	INV	165	04	04	227	02	2	289	93	.	351	95	=
042	08	08	104	52	EE	166	43	RCL	228	07	7	290	06	6	352	35	1/X
043	42	STO	105	01	1	167	08	08	229	00	0	291	06	6	353	42	STO
044	09	09	106	06	6	168	69	OP	230	00	0	292	07	7	354	01	01
045	99	PRT	107	02	2	169	06	06	231	01	1	293	65	×	355	04	4
046	91	R/S	108	04	4	170	95	=	232	05	5	294	43	RCL	356	01	1
(7) 047	42	STO	109	01	1	171	42	STO	233	03	3	295	11	11	357	00	0
048	09	09	110	03	3	172	16	16	234	02	2	296	55	÷	358	00	0
049	99	PRT	111	03	3	173	43	RCL	235	69	OP	297	03	3	359	00	0
050	91	R/S	112	00	0	174	09	09	236	02	02	298	07	7	360	00	0
(8) 051	76	LBL	113	69	OP	175	69	OP	237	03	3	299	00	0	361	69	OP
052	15	E	114	04	04	176	06	06	238	01	1	300	00	0	362	04	04
053	42	STO	115	43	RCL	177	03	3	239	01	1	301	69	OP	363	43	RCL
054	10	10	116	03	03	178	01	1	240	06	6	302	04	04	364	01	01
055	99	PRT	117	69	OP	179	00	0	241	04	4	303	43	RCL	365	69	OP
056	91	R/S	118	06	06	180	00	0	242	01	1	304	12	12	366	06	06
(9) 057	76	LBL	119	33	X^2	181	03	3	243	01	1	305	69	OP	(19) 367	65	×
058	16	A'	120	65	×	182	05	5	244	05	5	306	06	06	368	01	1
059	42	STO	121	03	3	183	01	1	245	03	3	307	22	INV	369	03	3
060	11	11	122	05	5	184	07	7	246	07	7	308	58	FIX	370	03	3
061	99	PRT	123	03	3	185	69	OP	247	69	OP	309	65	×	371	05	5

(Continued next page)

Program for TI-59 evaluates heat-transfer and power requirements for numerous reactor-agitator configurations

Step	Key	Code
372	01	1
373	07	7
374	01	1
375	03	3
376	69	OP
377	04	04
378	43	RCL
379	13	13
380	69	OP
381	06	06
382	65	×
383	02	2
384	07	7
385	03	3
386	00	0
387	01	1
388	06	6
389	03	3
390	07	7
391	69	OP
392	04	04
393	43	RCL
394	15	15
395	69	OP
396	06	06
397	95	=
398	42	STO
399	02	02
400	03	3
401	04	4
402	00	0
403	00	0
404	02	2
405	03	3
406	01	1
407	07	7
408	69	OP
409	04	04
410	43	RCL
411	02	02
412	69	OP
413	06	06
(20) 414	03	3
415	03	3
416	03	3
417	02	2
418	04	4
419	03	3
420	01	1
421	07	7
422	03	3
423	05	5
424	69	OP
425	00	00
426	69	OP
427	02	02
428	00	0
429	00	0
430	03	3
431	01	1
432	01	1
433	04	4

Step	Key	Code
434	03	3
435	05	5
436	00	0
437	00	0
438	69	OP
439	03	03
440	69	OP
441	05	05
442	06	6
443	00	0
444	00	0
445	32	X:T
446	43	RCL
447	16	16
448	77	GE
449	23	LNX
450	01	1
451	00	0
452	00	0
453	32	X:T
454	43	RCL
455	16	16
456	77	GE
457	28	LOG
458	23	LNX
459	65	×
460	93	.
461	04	4
462	04	4
463	02	2
464	04	4
465	94	+/-
466	85	+
467	02	2
468	93	.
469	07	7
470	03	3
471	07	7
472	03	3
473	61	GTO
474	25	CLR
475	76	LBL
476	28	LOG
477	23	LNX
478	65	×
479	93	.
480	02	2
481	01	1
482	07	7
483	08	8
484	08	8
485	94	+/-
486	85	+
487	01	1
488	93	.
489	06	6
490	09	9
491	00	0
492	07	7
493	61	GTO
494	25	CLR
495	76	LBL

Step	Key	Code
496	23	LNX
497	93	.
498	09	9
499	07	7
500	06	6
501	00	0
502	05	5
503	61	GTO
504	30	TAN
505	76	LBL
506	25	CLR
507	95	=
508	22	INV
509	23	LNX
510	65	×
511	93	.
512	07	7
513	02	2
514	03	3
515	95	=
516	76	LBL
517	30	TAN
518	42	STO
519	05	05
520	99	PRT
(21) 521	65	×
522	53	(
523	43	RCL
524	14	14
525	85	+
526	01	1
527	54	)
528	69	OP
529	04	04
530	03	3
531	01	1
532	03	3
533	02	2
534	04	4
535	00	0
536	00	0
537	00	0
538	03	3
539	02	2
540	69	OP
541	01	01
542	02	2
543	01	1
544	00	0
545	00	0
546	03	3
547	07	7
548	04	4
549	01	1
550	03	3
551	05	5
552	69	OP
553	02	02
554	01	1
555	04	4
556	02	2
557	04	4

Step	Key	Code
558	03	3
559	01	1
560	01	1
561	07	7
562	03	3
563	06	6
564	69	OP
565	03	03
566	69	OP
567	05	05
568	43	RCL
569	14	14
570	65	×
571	43	RCL
572	03	03
573	45	Y^X
574	05	5
575	65	×
576	43	RCL
577	04	04
578	45	Y^X
579	03	3
580	65	×
581	43	RCL
582	07	07
583	65	×
584	06	6
585	93	.
586	06	6
587	07	7
588	52	EE
589	07	7
590	94	+/-
591	95	=
592	42	STO
593	06	06
594	22	INV
595	52	EE
596	03	3
597	04	4
598	00	0
599	00	0
600	03	3
601	00	0
602	01	1
603	07	7
604	69	OP
605	04	04
606	43	RCL
607	06	06
608	94	+/-
609	69	OP
610	06	06
611	02	2
612	03	3
613	04	4
614	00	0
615	03	3
616	03	3
617	04	4
618	00	0
619	69	OP

Step	Key	Code
620	04	04
621	43	RCL
622	06	06
623	55	÷
624	02	2
625	05	5
626	05	5
627	00	0
628	95	=
629	69	OP
630	06	06
(22) 631	69	OP
632	00	00
633	01	1
634	07	7
635	02	2
636	01	1
637	02	2
638	01	1
639	01	1
640	07	7
641	01	1
642	05	5
643	69	OP
644	02	02
645	03	3
646	07	7
647	02	2
648	04	4
649	04	4
650	02	2
651	01	1
652	07	7
653	00	0
654	00	0
655	69	OP
656	03	03
657	69	OP
658	05	05
659	03	3
660	07	7
661	03	3
662	05	5
663	01	1
664	03	3
665	03	3
666	01	1
667	03	3
668	06	6
669	69	OP
670	02	02
671	02	2
672	01	1
673	01	1
674	07	7
675	03	3
676	05	5
677	00	0
678	00	0
679	00	0
680	00	0
681	69	OP

Step	Key	Code
682	03	03
683	02	2
684	03	3
685	01	1
686	07	7
687	01	1
688	03	3
689	03	3
690	07	7
691	00	0
692	00	0
693	69	OP
694	01	01
695	01	1
696	04	4
697	03	3
698	07	7
699	04	4
700	01	1
701	06	6
702	05	5
703	03	3
704	06	6
705	69	OP
706	04	04
707	69	OP
708	05	05
709	43	RCL
710	02	02
711	75	-
712	43	RCL
713	06	06
714	95	=
715	99	PRT
716	98	ADV
717	98	ADV
718	98	ADV
719	98	ADV
(23) 720	01	1
721	22	INV
722	44	SUM
723	19	19
724	43	RCL
725	19	19
726	59	INT
727	32	X:T
728	00	0
729	67	EQ
730	91	R/S
731	87	IFF
732	01	01
733	85	+
734	86	STF
735	01	01
736	43	RCL
737	17	17
738	75	-
739	43	RCL
740	04	04
741	95	=
742	55	÷
743	43	RCL

(continued) Table I

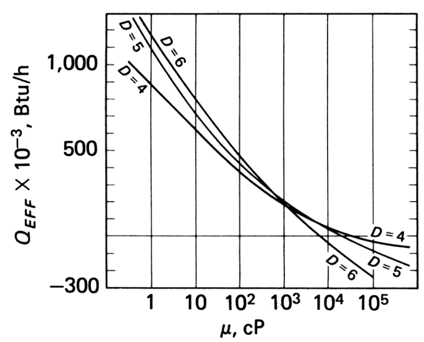
Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
744	19	19	748	76	LBL	752	44	SUM	756	61	GTO	760	01	1	764	69	OP
745	95	=	749	85	+	753	04	04	757	53	(	761	42	STO	765	00	00
746	42	STO	750	43	RCL	754	43	RCL	758	76	LBL	762	19	19	766	91	R/S
747	18	18	751	18	18	755	15	15	759	91	R/S	763	25	CLR			

Notes: See Table II, "User instructions," for further explanations. (1) Enter impeller diameter, D. (2) Enter agitator speed, N, or initial agitator speed to be used in chain calculation, N_1. (3) Enter final agitator speed to be used in chain calculation, N_2. (4) Enter number of agitator speeds to be used in chain calculation, n. (5) Enter density, ρ. (6) Enter bulk-liquid viscosity, μ. (7) Enter wall viscosity, μ_w. (8) Enter specific heat, C_p. (9) Enter thermal conductivity, k. (10) Enter heat-transfer coefficient, H_o. (11) Enter vessel diameter, T. (12) Enter heat-transfer area, A. (13) Enter number of turbines, β. (14) Enter log mean temperature difference, Δt. (15) Recall and print Δt, D, N, μ, and μ_w, then calculate and print N_{Re}. (16) Recall and print C_p and k, then calculate and print N_{Pr}. (17) Calculate $(\mu/\mu_w)^{0.24}$, $N_{Re}^{0.667}$, and k/T, then calculate and print h_i. (18) Calculate $1/h_i$ and $1/H_o$, then calculate and print U. (19) Calculate and print Q_{HE}. (20) Calculate and print N_P. (21) Calculate and print Q_{ME}, then convert it to P, in units of horsepower, and print P. (22) Calculate and print Q_{EFF}. (23) In a chain calculation, calculate the next speed to be used and repeat Steps 100-719 for the new speed; continue for a total of n iterations; stop program when appropriate.

User instructions for reactor-agitator optimization program **Table II**

Step	Procedure	Press	Display
1	Partition memory-storage area into 20 data registers and 800 program locations	CLR 2 2nd OP 17	799.19
2	Enter program as listed in Table I, or read program from cards if previously recorded		
3	Enter data, in any order, if different from what is stored in memory:		
3a	Enter impeller dia., D	A	Value entered for D is displayed and printed
$3b_1$	Enter agitator speed, N, or initial agitator speed to be used in chain calculation, N_1	B	N or N_1 is displayed and printed
$3b_2$*	Enter final agitator speed to be used in chain calculation, N_2	R/S	N_2 is displayed and printed
$3b_3$*	Enter no. of agitator speeds to be used in chain calculation, n	R/S	n is displayed and printed
3c	Enter density, ρ	C	ρ is displayed and printed
$3d_1$	Enter bulk-liquid viscosity, μ	D	μ is displayed and printed
$3d_2$†	Enter wall viscosity, μ_w, if different from μ	R/S	μ_w is displayed and printed
3e	Enter specific heat, C_p	E	C_p is displayed and printed
$3f_1$	Enter thermal conductivity, k	A'	k is displayed and printed
$3f_2$‡	Enter heat-transfer coefficient, H_o, if not 100 Btu/(h)(ft²)(°F)	R/S	H_o is displayed and printed
3g	Enter vessel dia., T	B'	T is displayed and printed
3h	Enter heat-transfer area, A	C'	A is displayed and printed
3i	Enter no. of turbines, β	D'	β is displayed and printed
4	Enter log mean temperature difference, Δt, (+) if cooling, (−) if heating	E'	Δt is displayed and printed Calculations proceed Data and results are printed in the following order: 1. D 2. N 3. ρ 4. μ 5. μ_w 6. N_{Re} 7. k 8. T 9. h_i 10. U 11. A 12. Δt 13. Q_{HE} 14. N_P 15. β 16. Q_{ME} 17. P 18. Q_{EFF}
5	If new data input is desired to be maintained in memory, record on card side 4	CLR 4 2nd WRITE	4

* These steps are required only for chain calculations.
† If wall viscosity is not entered, the value for the bulk-liquid viscosity is automatically used.
‡ If no value for H_o is entered, it is assumed to be 100 Btu/(h)(ft²)(°F), and is reset to that value each time a new thermal conductivity, k, is entered.



Effective heat transfer vs. viscosity, as a function of impeller diameter, at optimum impeller speed Fig. 3

Q_{EFF} determined from actual measurements. If a significant difference is found, correct the area, A, as follows:

$$A' = A[Q_{EFF(determined)}/Q_{EFF(calculated)}]$$

5. Rerun the program, using A' for A. Within reasonable limits, the heat-transfer calculation should now be more accurate, as the parameters have been varied

If the above approaches do not yield acceptable accuracies in a given application, regrettably it's back to the basics. (See the reference given below.)

Example: optimizing agitator design

Suppose we want to determine the agitator design for a 7,500-gal reactor that will optimally cool a wide range of viscous materials. The system properties are: $T = 8.5$ ft; $A = 420$ ft^2; $\beta = 4$; $\Delta t = +45$°F; $\rho = 75.2488$ lb/ft^3; $C_p = 0.4095$ Btu/(lb)(°F); and $k = 0.099$ Btu/(h)(ft^2)(°F). The following viscosities are expected to be encountered:

Bulk viscosity, cP	Wall viscosity, cP
1	1.3
10	15
150	300
3,000	5,000
50,000	75,000

The program was run for impeller diameters of 3, 3.5, 4, 4.5, 5, 5.5, and 6 ft, and for viscosities of 1, 10, 150, 3,000, and 50,000 cP. Families of curves, one for each viscosity level, showing Q_{EFF} vs. N for various agitator impeller diameters (the solid lines in Fig. 2, for $\mu = 10$ cP), were plotted. Inspection of the plots reveals that a 5-ft impeller operating at 40 rpm represents an operating point within about 5% of optimum for all viscosities from 1 to 3,000 cP.

In Fig. 2, Q_{EFF} is represented by the solid lines and is read from the scale on the left side of the plot. The bending of each curve through a maximum is caused by the mechanical energy input from agitation. For comparison, Q_{ME} is shown by the dashed lines, and its value is found on the right-hand scale. In addition, Q_{ME} is translated into power consumption, in horsepower, by using the scale to the right of the Q_{ME} scale.

After the optimum speed has been selected, Q_{EFF} vs. μ can be plotted for different diameters, as was done in Fig. 3. This figure indicates that viscosities of up to about 20,000 cP could be processed with a 5-ft-dia. agitator configuration while at least the total mechanical heat of agitation could still be removed.

If one were to choose the 6-ft impeller, only a marginal improvement in heat transfer at low viscosities would result (perhaps 5%), while a 20% heat-transfer penalty would result at 3,000 cP. In addition, the upper viscosity limit would be reduced to only about 7,000 cP.

On the other hand, if the 4-ft impeller were chosen, higher-viscosity materials could be processed (up to about 40,000 cP) at a heat-transfer penalty of 10–30% in the low-viscosity region.

Final comments

This mathematical treatment of agitation power consumption rather closely predicts the actual measured agitator-power requirements after appropriate adjustments are made for motor efficiencies and gear-box and agitator-seal frictional losses. Generally, a ±15% agreement is found, except for cases where gas or vapor bubbles exist.

The reactor sizes evaluated include 2,000, 3,000, 5,000 and 20,000 gal. The viscosities encountered during the data-gathering trials ranged from 10 to 40,000 cP. However, because the reference for the relationships on which this program is based covered viscosities up to 100,000 cP, this program, too, should be valid to 100,000 cP.

There have been fewer opportunities to evaluate the heat-transfer portion of the program. In one case, however, a 20,000-gal reactor was investigated, and the calculated agitator power and amount of heat transferred both agreed to within 5% of the measured values.

For HP users

A listing for the HP version of the program is shown in Table III. User instructions are listed in Table IV. Operation is similar to the TI version.

Program listing for HP version Table III

Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	023	R/S	51
002	DSP1	-63 01	024	*LBLa	21 16 11
003	STO3	35 03	025	STOC	35 13
004	R/S	51	026	1	01
005	*LBLB	21 12	027	0	00
006	STO4	35 04	028	0	00
007	STOA	35 11	029	STO0	35 00
008	RCL4	36 04	030	RCLC	36 13
009	R/S	51	031	R/S	51
010	STOA	35 11	032	STO0	35 00
011	R/S	51	033	R/S	51
012	*LBLC	21 13	034	*LBLb	21 16 12
013	STO7	35 07	035	STOD	35 14
014	R/S	51	036	R/S	51
015	*LBLD	21 14	037	*LBLc	21 16 13
016	STO6	35 06	038	STOE	35 15
017	STO5	35 05	039	R/S	51
018	R/S	51	040	*LBLd	21 16 14
019	STO9	35 09	041	STO1	35 01
020	R/S	51	042	R/S	51
021	*LBLE	21 15	043	*LBLe	21 16 15
022	STOB	35 12	044	STO2	35 02

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
045	*LBL1	21 11	081	4	04	117	PRTX	-14	153	STO5	35 05	189	RCL3	36 03
046	RCL3	36 03	082	×	-35	118	×	-35	154	*LBL3	21 03	190	5	05
047	PRTX	-14	083	RCLB	36 12	119	PRTX	-14	155	2	02	191	Y^x	31
048	X^2	53	084	RCL6	36 06	120	STO6	35 06	156	.	-62	192	×	-35
049	RCL4	36 04	085	×	-35	121	6	06	157	7	07	193	RCL4	36 04
050	PRTX	-14	086	2	02	122	0	00	158	3	03	194	3	03
051	×	-35	087	.	-62	123	0	00	159	7	07	195	Y^x	31
052	RCL7	36 07	088	4	04	124	RCL5	36 05	160	3	03	196	×	-35
053	PRTX	-14	089	×	-35	125	X>Y?	16-34	161	ENT↑	-21	197	RCL7	36 07
054	×	-35	090	RCLC	36 13	126	GTO2	22 02	162	.	-62	198	×	-35
055	RCL8	36 08	091	÷	-24	127	1	01	163	4	04	199	6	06
056	PRTX	-14	092	.	-62	128	0	00	164	4	04	200	.	-62
057	÷	-24	093	3	03	129	0	00	165	2	02	201	6	06
058	2	02	094	3	03	130	X>Y?	16-34	166	4	04	202	7	07
059	4	04	095	3	03	131	GTO3	22 03	167	*LBL4	21 04	203	EEX	-23
060	.	-62	096	Y^x	31	132	1	01	168	RCL5	36 05	204	CHS	-22
061	3	03	097	×	-35	133	.	-62	169	LN	32	205	7	07
062	×	-35	098	RCL8	36 08	134	6	06	170	×	-35	206	×	-35
063	STO5	35 05	099	RCL9	36 09	135	9	09	171	CHS	-22	207	PRTX	-14
064	RCL9	36 09	100	÷	-24	136	6	06	172	+	-35	208	ENT↑	-21
065	PRTX	-14	101	.	-62	137	7	07	173	e^x	33	209	ENT↑	-21
066	RCL5	36 05	102	2	02	138	ENT↑	-21	174	.	-62	210	2	02
067	PRTX	-14	103	4	04	139	.	-62	175	2	02	211	5	05
068	.	-62	104	Y^x	31	140	2	02	176	7	07	212	5	05
069	6	06	105	×	-35	141	1	01	177	3	03	213	0	00
070	6	06	106	PRTX	-14	142	7	07	178	×	-35	214	÷	-24
071	7	07	107	1/X	52	143	8	08	179	*LBL5	21 05	215	PRTX	-14
072	Y^x	31	108	RCL0	36 00	144	8	08	180	STOA	35 11	216	R↓	-31
073	RCLC	36 13	109	1/X	52	145	GTO4	22 04	181	PRTX	-14	217	CHS	-22
074	PRTX	-14	110	+	-55	146	*LBL2	21 02	182	RCL1	36 01	218	RCL6	36 06
075	×	-35	111	1/X	52	147	.	-62	183	1	01	219	+	-55
076	RCLD	36 14	112	PRTX	-14	148	9	09	184	+	-55	220	PRTX	-14
077	PRTX	-14	113	RCLE	36 15	149	7	07	185	PRTX	-14	221	SPC	16-11
078	÷	-24	114	PRTX	-14	150	6	06	186	1	01	222	R/S	51
079	.	-62	115	×	-35	151	0	00	187	−	-45			
080	4	04	116	RCL2	36 02	152	5	05	188	×	-35			

User instructions for the HP version — Table IV

	Key
Enter impeller diameter *D*, ft	A
Enter agitator *N*, rpm	B
Enter liquid density ρ, lb/ft^3	C
Enter viscosity μ, cP	D
Enter specific heat C_p, Btu/(lb)(°F)	E
Enter thermal conductivity *K*, Btu/(h)(ft)(°F)	a
Enter vessel diameter *T*, ft	b
Enter heat transfer area *A*, ft^2	c
Enter number of turbines β	d
Enter log mean temperature Δt, °F	e

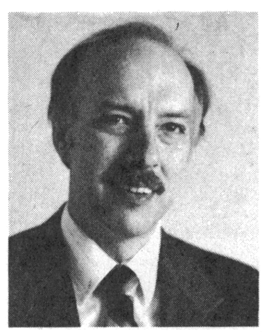
Printed output will be as follows (this is in the same order as the TI output):

1. *D*, Impeller diameter, ft
2. *N*, Impeller speed, rpm
3. ρ, Liquid density, lb/ft^3
4. μ, Liquid viscosity, cP
5. μ_w, Wall viscosity, cP
6. N_{Re}, Reynolds number
7. *k*, Thermal conductivity, Btu/(h)(ft)(°F)
8. *T*, Vessel diameter, ft
9. h_i, Inside film coefficient, Btu/(h)(ft^2)(°F)
10. *U*, Overall heat transfer coefficient, Btu/(h)(ft^2)(°F)
11. *A*, Heat transfer area, ft^2
12. Δ_t, Log mean temperature difference, °F
13. Q_{HE}, Heat transferred, Btu/h
14. N_p, Power number
15. β, Number of turbines
16. Q_{ME}, Mechanical heat of agitation, Btu/h
17. *P*, Agitator power consumption, hp
18. Q_{EFF}, Effective heat removal, Btu/h

Reference

Uhl, V. W. and Gray, J. B., "Mixing—Theory and Practice," Vol. 1, Academic Press, New York, 1966, Chapters 3 and 5.

The authors



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Section VII
Engineering Economics

Estimating cash flows for construction projects

Estimates of monthly cash-flow requirements for a construction project can be valuable to both client and contractor. These can be calculated rapidly by means of this TI-59 program.

George F. Poland, *Aberthaw Construction Co.*

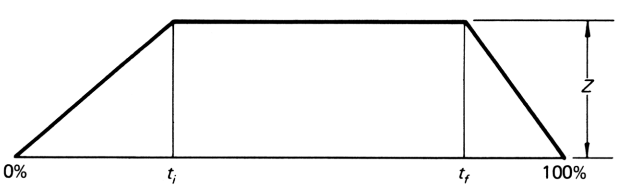
☐ During the course of a construction project, it is important for the owner and contractor to be able to predict cash demands. The owner wishes to know when the money has to be spent, and the contractor needs to know how much cash has to be invested in the project.

A program for the TI-59 calculator and printer is presented that will project on a monthly basis the total cost to date of a job, the payments from the owner, the contractor's investment (which depends on the time lapse between billings and payments), and the interest costs for the contractor's investment.

S-curve basis for the program

The program is based on the S-curve approach to project planning. The work of most projects can be divided into three major periods: the first, increasing manpower requirements; the second, constant requirements; the third, declining requirements. Plots of work-completion-percentage vs. time-lapse-percentage come out as the familiar S-curve. The shape of the manpower curve is a trapezoid.

A mathematical explanation of the S-curve by Gates and Scarpa* can be summarized by the diagram:



Here, Z = maximum rate of manpower; t_i = end of accelerating manpower period, %; and t_f = beginning of declining manpower period, %. Because the trapezoid area equals 100%, $Z = 200/[100 + (t_f - t_i)]$.

*Gates, M., and Scarpa, A., Conceptual RMC/Time Synthesis, *J. of the Construction Div.*, American Soc. of Construction Engineers, Vol. 102, No. CO2, Proc. Paper 12181, June 1976, pp. 307-323.

Values of 50% for t_i and 75% for t_f "seem to fit" most construction projects. Therefore, $Z = 1.6$, which means that the maximum crew size is equal to 1.6 times the average crew size.

These values plotted in the S-curve will show that only 40% of the work will be completed after a 50% time lapse, but that 80% will be finished at the 75% time mark. Thereafter, the rate of work completion decelerates to arrive at 100% completion at 100% of the scheduled construction period.

How the program works

As an example, assume that a $1-million project is to be completed within 10 months, and that 95% of the incurred costs will be paid to the contractor, with a two-month delay between billings and payments. The short-term borrowing cost for the contractor is 21% interest. The contractor expects that the size of the working crew will increase until the 50% point in time, then begin to decline at the 75% mark.

With the program listed in Table I in the calculator, enter 75 (t_f) and press the **A** key. Enter 50 (t_i) and press **R/S**. Enter 10 (number of scheduled construction months) and press **R/S** again. Enter 1,000,000 (the cost of the project) and press **B**. Enter 95 (% paid) and press **R/S**. Enter 2 (number of months delay in payments) and press **R/S** again. Enter 21 (% interest) and press **C**. Finally, press **D** (start) and **E** (clear).

The program will list the input data and print out on a month-to-month basis the following:

Month number, *MO*.

The estimated percentage of work completed, *%C*.

Costs to date at the end of the month, *COT*.

The total paid to the contractor, *TP*.

The total investment of the contractor, *INV*.

The interest cost per month for the contractor's investment, *INT*.

The total of all interest costs to date, ΣINT.

The printout for this example is listed per month in Table II.

Other possibilities can be simulated

Variations in the project can be readily examined by means of the program. For example, if the time delay between billings and payments were shortened by one month, the amount the contractor would need to invest would fall from $340,000 to $188,000, and interest costs would decline from $39,375 to $21,875. If 10% of the

Originally published August 9, 1982.

On monthly basis, program calculates project costs, total paid to contractor, contractor's investment, and interest cost of investment

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	063	05	05	126	01	1	189	69	OP	252	95	=	315	39	COS
001	35	1/X	064	54	)	127	42	STO	190	04	04	253	42	STO	316	53	(
002	43	RCL	065	33	X^2	128	07	07	191	32	X⇌T	254	05	05	317	43	RCL
003	04	04	066	55	÷	129	42	STO	192	69	OP	255	43	RCL	318	00	00
004	65	×	067	53	(	130	09	09	193	06	06	256	02	02	319	85	+
005	43	RCL	068	01	1	131	42	STO	194	91	R/S	257	32	X⇌T	320	01	1
006	05	05	069	00	0	132	10	10	195	42	STO	258	43	RCL	321	09	9
007	33	X^2	070	00	0	133	00	0	196	10	10	259	05	05	322	54	)
008	55	÷	071	75	-	134	42	STO	197	32	X⇌T	260	22	INV	323	42	STO
009	02	2	072	43	RCL	135	12	12	198	01	1	261	77	GE	324	13	13
010	55	÷	073	01	01	136	91	R/S	199	06	6	262	35	1/X	325	53	(
011	43	RCL	074	54	)	137	42	STO	200	02	2	263	43	RCL	326	43	RCL
012	02	02	075	54	)	138	03	03	201	07	7	264	01	01	327	00	00
013	95	=	076	54	)	139	32	X⇌T	202	04	4	265	32	X⇌T	328	75	-
014	42	STO	077	42	STO	140	03	3	203	05	5	266	43	RCL	329	43	RCL
015	06	06	078	06	06	141	01	1	204	69	OP	267	05	05	330	10	10
016	61	GTO	079	61	GTO	142	03	3	205	04	04	268	22	INV	331	85	+
017	45	Y^X	080	45	Y^X	143	00	0	206	32	X⇌T	269	77	GE	332	01	1
018	76	LBL	081	76	LBL	144	69	OP	207	69	OP	270	34	√X	333	09	9
019	34	√X	082	37	P/R	145	04	04	208	06	06	271	71	SBR	334	54	)
020	43	RCL	083	01	1	146	32	X⇌T	209	91	R/S	272	33	X^2	335	42	STO
021	04	04	084	00	0	147	69	OP	210	76	LBL	273	76	LBL	336	14	14
022	65	×	085	00	0	148	06	06	211	13	C	274	45	Y^X	337	43	RCL
023	53	(	086	42	STO	149	53	(	212	42	STO	275	43	RCL	338	06	06
024	43	RCL	087	06	06	150	02	2	213	12	12	276	00	00	339	65	×
025	05	05	088	43	RCL	151	00	0	214	32	X⇌T	277	32	X⇌T	340	43	RCL
026	75	-	089	03	03	152	00	0	215	02	2	278	03	3	341	07	07
027	43	RCL	090	85	+	153	55	÷	216	04	4	279	00	0	342	55	÷
028	02	02	091	43	RCL	154	53	(	217	03	3	280	03	3	343	01	1
029	55	-	092	10	10	155	01	1	218	01	1	281	02	2	344	00	0
030	02	2	093	85	+	156	00	0	219	03	3	282	69	OP	345	00	0
031	54	)	094	01	1	157	00	0	220	07	7	283	04	04	346	95	=
032	54	)	095	95	=	158	85	+	221	69	OP	284	32	X⇌T	347	72	ST*
033	42	STO	096	32	X⇌T	159	43	RCL	222	04	04	285	69	OP	348	13	13
034	06	06	097	43	RCL	160	01	01	223	32	X⇌T	286	06	06	349	32	X⇌T
035	61	GTO	098	00	00	161	75	-	224	69	OP	287	43	RCL	350	01	1
036	45	Y^X	099	77	GE	162	43	RCL	225	06	06	288	06	06	351	05	5
037	76	LBL	100	90	LST	163	02	02	226	43	RCL	289	32	X⇌T	352	03	3
038	33	X^2	101	61	GTO	164	54	)	227	12	12	290	06	6	353	02	2
039	43	RCL	102	45	Y^X	165	54	)	228	55	÷	291	01	1	354	03	3
040	03	03	103	76	LBL	166	42	STO	229	01	1	292	01	1	355	07	7
041	32	X⇌T	104	11	A	167	04	04	230	02	2	293	05	5	356	69	OP
042	43	RCL	105	42	STO	168	91	R/S	231	95	=	294	69	OP	357	04	04
043	00	00	106	01	01	169	76	LBL	232	42	STO	295	04	04	358	32	X⇌T
044	77	GE	107	32	X⇌T	170	12	B	233	12	12	296	32	X⇌T	359	69	OP
045	37	P/R	108	00	0	171	42	STO	234	91	R/S	297	69	OP	360	06	06
046	53	(	109	03	3	172	07	07	235	76	LBL	298	06	06	361	01	1
047	01	1	110	69	OP	173	32	X⇌T	236	14	D	299	02	2	362	32	X⇌T
048	00	0	111	04	04	174	03	3	237	98	ADV	300	32	X⇌T	363	43	RCL
049	00	0	112	32	X⇌T	175	03	3	238	01	1	301	43	RCL	364	09	09
050	75	-	113	69	OP	176	01	1	239	42	STO	302	07	07	365	67	EQ
051	43	RCL	114	06	06	177	05	5	240	00	00	303	77	GE	366	28	LOG
052	04	04	115	91	R/S	178	69	OP	241	76	LBL	304	39	COS	367	73	RC*
053	55	÷	116	42	STO	179	04	04	242	24	CE	305	43	RCL	368	14	14
054	02	2	117	02	02	180	32	X⇌T	243	43	RCL	306	03	03	369	65	×
055	65	×	118	32	X⇌T	181	69	OP	244	00	00	307	32	X⇌T	370	43	RCL
056	53	(	119	00	0	182	06	06	245	55	÷	308	43	RCL	371	09	09
057	53	(	120	02	2	183	91	R/S	246	43	RCL	309	00	00	372	55	÷
058	01	1	121	69	OP	184	42	STO	247	03	03	310	22	INV	373	01	1
059	00	0	122	04	04	185	09	09	248	65	×	311	77	GE	374	00	0
060	00	0	123	32	X⇌T	186	32	X⇌T	249	01	1	312	28	LOG	375	00	0
061	75	-	124	69	OP	187	06	6	250	00	0	313	91	R/S	376	54	)
062	43	RCL	125	06	06	188	01	1	251	00	0	314	76	LBL	377	42	STO

Table I

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
378	08	08	395	54	)	412	43	RCL	429	02	2	446	04	4	463	91	R/S
379	32	X:T	396	42	STO	413	12	12	430	04	4	447	03	3	464	76	LBL
380	03	3	397	08	08	414	67	EQ	431	03	3	448	01	1	465	90	LST
381	07	7	398	32	X:T	415	28	LOG	432	01	1	449	03	3	466	01	1
382	03	3	399	02	2	416	43	RCL	433	03	3	450	07	7	467	00	0
383	03	3	400	04	4	417	08	08	434	07	7	451	69	OP	468	00	0
384	69	OP	401	03	3	418	65	×	435	69	OP	452	04	04	469	42	STO
385	04	04	402	01	1	419	43	RCL	436	04	04	453	32	X:T	470	09	09
386	32	X:T	403	04	4	420	12	12	437	32	X:T	454	69	OP	471	61	GTO
387	69	OP	404	02	2	421	55	÷	438	69	OP	455	06	06	472	45	Y^x
388	06	06	405	69	OP	422	01	1	439	06	06	456	76	LBL	473	76	LBL
389	53	(	406	04	04	423	00	0	440	43	RCL	457	28	LOG	474	15	E
390	73	RC*	407	32	X:T	424	00	0	441	11	11	458	98	ADV	475	47	CMS
391	13	13	408	69	OP	425	95	=	442	32	X:T	459	69	OP	476	25	CLR
392	75	-	409	06	06	426	44	SUM	443	07	7	460	20	20	477	91	R/S
393	43	RCL	410	00	0	427	11	11	444	07	7	461	61	GTO			
394	08	08	411	32	X:T	428	32	X:T	445	02	2	462	24	CE			

Output for example case gives monthly breakdown of costs **Table II**

75.	2	1.	MO	2.	MO	3.	MO	4.	MO
50.	1	1.6	%C	6.4	%C	14.4	%C	25.6	%C
10.	NM	16000.	COT	64000.	COT	144000.	COT	256000.	COT
1000000.	PC	0.	TP	0.	TP	15200.	TP	60800.	TP
95.	%	16000.	INV	64000.	INV	128800.	INV	195200.	INV
2.	DLY	280.	INT	1120.	INT	2254.	INT	3416.	INT
21.	INT	280.	ΣINT	1400.	ΣINT	3654.	ΣINT	7070.	ΣINT
a.		b.		c.		d.		e.	

5.	MO	6.	MO	7.	MO	8.	MO	9.	MO
40.	%C	56.	%C	72.	%C	87.2	%C	96.8	%C
400000.	COT	560000.	COT	720000.	COT	872000.	COT	968000.	COT
136800.	TP	243200.	TP	380000.	TP	532000.	TP	684000.	TP
263200.	INV	316800.	INV	340000.	INV	340000.	INV	284000.	INV
4606.	INT	5544.	INT	5950.	INT	5950.	INT	4970.	INT
11676.	ΣINT	17220.	ΣINT	23170.	ΣINT	29120.	ΣINT	34090.	ΣINT
f.		g.		h.		i.		j.	

10.	MO	11.	MO	12.	MO	13.	MO	14.	MO
100.	%C	100.	%C	100.	%C	100.	%C	100.	%C
1000000.	COT	1000000.	COT	1000000.	COT	1000000.	COT	1000000.	COT
828400.	TP	919600.	TP	950000.	TP	1000000.	TP	1000000.	TP
171600.	INV	80400.	INV	50000.	INV	0.	INV	0.	INV
3003.	INT	1407.	INT	875.	INT	0.	INT	0.	INT
37093.	ΣINT	38500.	ΣINT	39375.	ΣINT	39375.	ΣINT	39375.	ΣINT
k.		l.		m.		n.		o.	

cost of the project ($100,000) represents the contractor's profit, the shortening of the payment-lapse time to one month would increase the contractor's return on investment to 53% from 27%.

Another useful simulation would be to determine how much of the work ought to be completed at the end of each month. If the S curve for the actual work completed and the S curve for the work that should have been accomplished do not agree reasonably well, this will be a signal that decisive action needs to be taken to really control costs.

For HP-67/97 users

The HP version closely follows the TI program. Table III offers the HP program listing, and Table IV contains user instructions and the example for the HP version.

Program listing for HP version **Table III**

Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	069	*LBL5	21 05
002	CLRG	16-53	070	RCL0	36 00
003	P⇄S	16-51	071	PRTX	-14
004	CLRG	16-53	072	RCL6	36 06
005	STO7	35 07	073	PRTX	-14
006	R↓	-31	074	GTO4	22 04
007	STO3	35 03	075	*LBL1	21 01
008	R↓	-31	076	RCL4	36 04
009	STO2	35 02	077	RCL5	36 05
010	R↓	-31	078	X²	53
011	STO1	35 01	079	2	02
012	R/S	51	080	÷	-24
013	STOC	35 13	081	RCL2	36 02
014	R↓	-31	082	÷	-24
015	STOA	35 11	083	×	-35
016	R↓	-31	084	STO6	35 06
017	STO9	35 09	085	GTO5	22 05
018	RCL1	36 01	086	*LBL2	21 02
019	PRTX	-14	087	RCL4	36 04
020	RCL2	36 02	088	RCL5	36 05
021	PRTX	-14	089	RCL2	36 02
022	RCL3	36 03	090	2	02
023	PRTX	-14	091	÷	-24
024	RCL7	36 07	092	-	-45
025	PRTX	-14	093	×	-35
026	RCL9	36 09	094	STO6	35 06
027	PRTX	-14	095	GTO5	22 05
028	RCLA	36 11	096	*LBL3	21 03
029	PRTX	-14	097	RCL3	36 03
030	RCLC	36 13	098	RCL0	36 00
031	PRTX	-14	099	X=Y?	16-33
032	SPC	16-11	100	GTO6	22 06
033	1	01	101	X>Y?	16-34
034	0	00	102	GTO6	22 06
035	0	00	103	RCLE	36 15
036	STOE	35 15	104	RCL5	36 05
037	RCL1	36 01	105	-	-45
038	+	-55	106	X²	53
039	RCL2	36 02	107	RCLE	36 15
040	-	-45	108	RCL1	36 01
041	1/X	52	109	-	-45
042	2	02	110	÷	-24
043	0	00	111	RCL4	36 04
044	0	00	112	2	02
045	×	-35	113	÷	-24
046	STO4	35 04	114	×	-35
047	RCLC	36 13	115	CHS	-22
048	1	01	116	RCLE	36 15
049	2	02	117	+	-55
050	÷	-24	118	STO6	35 06
051	STOC	35 13	119	GTO5	22 05
052	1	01	120	*LBL6	21 06
053	STO0	35 00	121	RCLE	36 15
054	*LBL9	21 09	122	STO6	35 06
055	RCL0	36 00	123	RCL3	36 03
056	RCL3	36 03	124	RCLA	36 11
057	÷	-24	125	+	-55
058	RCLE	36 15	126	1	01
059	×	-35	127	+	-55
060	STO5	35 05	128	RCL0	36 00
061	RCL2	36 02	129	X=Y?	16-33
062	X>Y?	16-34	130	GTO7	22 07
063	GTO1	22 01	131	X>Y?	16-34
064	RCL5	36 05	132	GTO7	22 07
065	RCL1	36 01	133	GTO5	22 05
066	X>Y?	16-34	134	*LBL7	21 07
067	GTO2	22 02	135	RCLE	36 15
068	GTO3	22 03			

(Continued) Table III

Step	Key	Code	Step	Key	Code
136	STO9	35 09	180	P⇄S	16-51
137	GTO5	22 05	181	RCL8	36 08
138	*LBL4	21 04	182	-	-45
139	5	05	183	STO8	35 08
140	RCLA	36 11	184	PRTX	-14
141	-	-45	185	RCLC	36 13
142	1	01	186	X=0?	16-43
143	0	00	187	GTO8	22 08
144	•+	-55	188	RCL8	36 08
145	STOI	35 46	189	RCLC	36 13
146	P⇄S	16-51	190	×	-35
147	RCL1	36 01	191	RCLE	36 15
148	STO0	35 00	192	÷	-24
149	RCL2	36 02	193	PRTX	-14
150	STO1	35 01	194	RCLB	36 12
151	RCL3	36 03	195	+	-55
152	STO2	35 02	196	STOB	35 12
153	RCL4	36 04	197	PRTX	-14
154	STO3	35 03	198	SPC	16-11
155	RCL5	36 05	199	RCL8	36 08
156	STO4	35 04	200	X=0?	16-43
157	P⇄S	16-51	201	R/S	51
158	RCL6	36 06	202	*LBL8	21 08
159	RCL7	36 07	203	1	01
160	×	-35	204	ST+0	35-55 00
161	RCLE	36 15	205	GTO9	22 09
162	÷	-24	206	PRTX	-14
163	P⇄S	16-51	207	RCLB	36 12
164	PRTX	-14	208	+	-55
165	STO5	35 05	209	STOB	35 12
166	P⇄S	16-51	210	PRTX	-14
167	RCL9	36 09	211	RCL8	36 08
168	1	01	212	RCLC	36 13
169	X=Y?	16-33	213	×	-35
170	GTO8	22 08	214	1	01
171	RCLi	36 45	215	0	00
172	RCL9	36 09	216	0	00
173	×	-35	217	X=0?	16-43
174	RCLE	36 15	218	R/S	51
175	÷	-24	219	*LBL8	21 08
176	STO8	35 08	220	1	01
177	PRTX	-14	221	ST+0	35-55 00
178	P⇄S	16-51	222	GTO9	22 09
179	RCL5	36 05	223	R/S	51

User instructions and example for HP version **Table IV**

Instruction	Key
Enter t_f-Beginning of "declining manpower" period	ENTER ↑
Enter t_i-End of "accelerating manpower" period	ENTER ↑
Enter number of scheduled construction months	ENTER ↑
Enter construction cost, $	A
Enter % paid	ENTER ↑
Enter number of months delay in payment	ENTER ↑
Enter interest rate, %	R/S

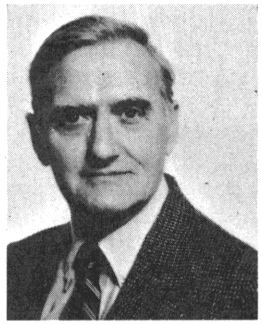
Output is the same as indicated in the original article.
Program stops when contractor has been paid in total.

(Continued) Table IV

```
     75.00 ENT↑
     50.00 ENT↑
     10.00 ENT↑
1000000.00 GSBA
     95.00 ENT↑
      2.00 ENT↑
     21.00 [illegible]
     75.00  ***
     50.00  ***
     10.00  ***
1000200.00  ***
     95.00  ***
      2.00  ***
     21.00  ***

      1.00  ***
      1.60  ***
  16000.00  ***
      0.00  ***
  16000.00  ***
    280.00  ***
    280.00  ***

      2.00  ***
      6.40  ***
  64000.00  ***
      0.00  ***
  64000.00  ***
   1120.00  ***
   1400.00  ***

      3.00  ***
     14.40  ***
 144000.00  ***
  15200.00  ***
 128800.00  ***
   2254.00  ***
   3654.00  ***

      4.00  ***
     25.60  ***
 256000.00  ***
  60800.00  ***
 195200.00  ***
   3416.00  ***
   7070.00  ***

      5.00  ***
     40.00  ***
 400000.00  ***
 136800.00  ***
 263200.00  ***
   4606.00  ***
  11676.00  ***

      6.00  ***
     56.00  ***
```

Nomenclature follows that of the original article.

The author



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Discounted-cash-flow rates of return for varying cash flows

Basing an economic analysis on a wide range of eventualities will enhance its reliability. Calculator programs make such a comprehensive analysis possible.

*Gordon W. Neal, Pacific Energy Consultants, Inc.**

☐ Uncertainty in economic evaluations can be reduced by examining alternative projects under many likely conditions. This was discussed in the article "Evaluating uncertainty in capital cost projections," *Chem. Eng.*, Sept. 6, 1982, p. 131.

There are two generally accepted bases for judging the economic attractiveness of projects: How much money will be generated, and how efficiently will the committed capital be used? A measure of the first is net present value (NPV), and of the second is discounted-cash-flow rate of return (DCFRR).

A TI-59 program for determining the NPV of an initial investment that is followed by a series of increasing or decreasing annual cash flows was presented in a Nov. 1, 1982 article. In the present article, two programs for the TI-59 are provided that calculate DCFRR for an initial investment that also is followed by a series of annual cash flows consisting of several components, each increasing or decreasing at a constant annual rate.

One program is designed for discrete compounding (Table I), the other for continuous compounding (Table II). Both include an option for after-tax or before-tax (e.g., government funded) modes. The after-tax modes are based on sum-of-years-digits (SOYD) depreciation.

The programs arrive at solutions via trial-and-error iteration, with successive calculations of NPV made with converging values of discount rate until the resulting value of NPV is nearly zero. When this point is reached, the corresponding discount rate—the DCFRR—is printed and displayed.

Program formulas

The general formula used in the programs is:

$$NPV = (C_1D_1 + C_2D_2 + \cdots + C_ND_N) + IR_TD - C_0 \qquad (1)$$

Here, NPV = net present value, in any monetary unit; $C_1, C_2 \ldots C_N$ = first-year cash flow components, in (positive) or out (negative); $D_1, D_2 \ldots D_N$ = discount factor corresponding to cash-flow component having same subscript; I = total initial investment; R_T = income tax rate; D = depreciation discount factor; and C_0 = net initial investment.

Cash-flow-component discount factors for continuous and discrete compounding are, respectively:

$$D_C = (1 - e^{-rn})/r \qquad (2)$$

$$D_D = [1 - (1 + r)^{-n}]/r \qquad (3)$$

Here, n = economic life, yr, and r = effective discount rate.

Expressions for effective discount rates with continuous and discrete compounding are, respectively:

$$r_C = R - i \qquad (4)$$

$$r_D = (R - i)/(1 + i) \qquad (5)$$

Here, R = selected discount rate, and i = annual rate at which cash flow component increases (positive) or decreases (negative).

The depreciation discount factor (based on continuous compounding and SOYD depreciation) is:

$$D = 2\,(RT' + e^{-RT'} - 1)/(RT')^2 \qquad (6)$$

Here, $T' = T + 1/2$, and T = depreciable life, yr.

Preparing and entering data

User instructions are given in Table III. The differences between the input data printed and the values displayed arise because common values in the display are combined to eliminate the need for repetitive calculations in the iterations. Note that the sequence for entering data is altered by the tax mode selected.

In the after-tax mode, the initial investment, C_0, should be adjusted to reflect such items as investment tax credit and energy tax credit. In the before-tax mode, the full initial investment is used.

In the after-tax mode, first-year cash flow components, C_1, C_2, etc., are multiplied by $(1 - R_T)$ to arrive at input values. No adjustments are made with the before-tax mode. Components of cash flow into the project (sales, reduced costs, etc.) have positive signs, and those flowing out (expenses, higher costs, etc.) have negative signs.

Depreciation is applied to only the after-tax mode. The expression $I\,R_T$ consists of the full initial investment (without credits) multiplied by the tax rate.

Program features

In each program, Flag 1 is set by the user when the before-tax mode is desired. When no flags are set, the program follows the after-tax mode.

*To meet the author, see p. 258.

Originally published December 27, 1982.

Program calculates discounted-cash-flow rate of return with discrete compounding **Table I**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
000	76	LBL	063	57	57	126	76	LBL	189	54	)	205	43	RCL	221	61	GTO
001	11	A	064	42	STO	127	24	CE	190	55	÷	206	56	56	222	30	TAN
002	58	FIX	065	53	53	128	87	IFF	191	02	2	207	85	+	223	76	LBL
003	09	09	066	76	LBL	129	01	01	192	95	=	208	43	RCL	224	39	COS
004	47	CMS	067	33	X^2	130	45	Y^x	193	48	EXC	209	55	55	225	43	RCL
005	42	STO	068	75	-	131	43	RCL	194	55	55	210	54	)	226	55	55
006	59	59	069	01	1	132	55	55	195	42	STO	211	55	÷	227	65	×
007	99	PRT	070	95	=	133	65	×	196	56	56	212	02	2	228	01	1
008	91	R/S	071	42	STO	134	43	RCL	197	00	0	213	95	=	229	00	0
009	42	STO	072	52	52	135	46	46	198	42	STO	214	48	EXC	230	00	0
010	58	58	073	43	RCL	136	95	=	199	50	50	215	55	55	231	95	=
011	99	PRT	074	55	55	137	42	STO	200	61	GTO	216	42	STO	232	58	FIX
012	91	R/S	075	75	-	138	45	45	201	30	TAN	217	54	54	233	01	01
013	99	PRT	076	73	RC*	139	33	X^2	202	76	LBL	218	00	0	234	99	PRT
014	65	×	077	53	53	140	35	1/X	203	23	LNX	219	42	STO	235	98	ADV
015	02	2	078	95	=	141	65	×	204	53	(	220	50	50	236	91	R/S
016	95	=	079	55	÷	142	53	(									
017	98	ADV	080	53	(	143	43	RCL									
018	42	STO	081	01	1	144	45	45									
019	57	57	082	85	+	145	85	+									
020	42	STO	083	73	RC*	146	24	CE									
021	00	00	084	53	53	147	94	+/-									
022	87	IFF	085	54	)	148	22	INV									
023	01	01	086	95	=	149	23	LNX									
024	38	SIN	087	42	STO	150	75	-									
025	91	R/S	088	51	51	151	01	1									
026	99	PRT	089	53	(	152	54	)									
027	65	×	090	01	1	153	65	×									
028	02	2	091	75	-	154	43	RCL									
029	95	=	092	53	(	155	47	47									
030	42	STO	093	01	1	156	95	=									
031	47	47	094	85	+	157	44	SUM									
032	91	R/S	095	43	RCL	158	50	50									
033	99	PRT	096	51	51	159	76	LBL									
034	85	+	097	54	)	160	45	Y^x									
035	93	.	098	45	Y^x	161	93	.									
036	05	5	099	43	RCL	162	01	1									
037	95	=	100	58	58	163	32	X⇌T									
038	42	STO	101	94	+/-	164	43	RCL									
039	46	46	102	54	)	165	50	50									
040	98	ADV	103	55	÷	166	75	-									
041	76	LBL	104	43	RCL	167	43	RCL									
042	38	SIN	105	51	51	168	59	59									
043	91	R/S	106	65	×	169	95	=									
044	99	PRT	107	73	RC*	170	42	STO									
045	72	ST*	108	52	52	171	49	49									
046	00	00	109	95	=	172	50	I×I									
047	97	DSZ	110	44	SUM	173	22	INV									
048	00	00	111	50	50	174	77	GE									
049	38	SIN	112	01	1	175	39	COS									
050	98	ADV	113	32	X⇌T	176	00	0									
051	93	.	114	43	RCL	177	32	X⇌T									
052	02	2	115	52	52	178	43	RCL									
053	05	5	116	67	EQ	179	49	49									
054	42	STO	117	24	CE	180	22	INV									
055	55	55	118	02	2	181	77	GE									
056	93	.	119	22	INV	182	23	LNX									
057	05	5	120	44	SUM	183	53	(									
058	42	STO	121	53	53	184	43	RCL									
059	54	54	122	43	RCL	185	55	55									
060	76	LBL	123	53	53	186	85	+									
061	30	TAN	124	61	GTO	187	43	RCL									
062	43	RCL	125	33	X^2	188	54	54									

DCFRR program with continuous compounding **Table II**

Step	Key	Code	Step	Key	Code	Step	Key	Code
000	76	LBL	040	93	.	080	55	55
001	11	A	041	05	5	081	75	-
002	58	FIX	042	95	=	082	73	RC*
003	09	09	043	42	STO	083	53	53
004	47	CMS	044	46	46	084	54	)
005	99	PRT	045	98	ADV	085	65	×
006	55	÷	046	76	LBL	086	43	RCL
007	91	R/S	047	38	SIN	087	59	59
008	99	PRT	048	91	R/S	088	95	=
009	42	STO	049	99	PRT	089	42	STO
010	59	59	050	72	ST*	090	51	51
011	95	=	051	00	00	091	35	1/X
012	42	STO	052	97	DSZ	092	65	×
013	58	58	053	00	00	093	53	(
014	91	R/S	054	38	SIN	094	01	1
015	99	PRT	055	98	ADV	095	75	-
016	65	×	056	93	.	096	43	RCL
017	02	2	057	02	2	097	51	51
018	95	=	058	05	5	098	94	+/-
019	42	STO	059	42	STO	099	22	INV
020	57	57	060	55	55	100	23	LNX
021	42	STO	061	93	.	101	54	)
022	00	00	062	05	5	102	65	×
023	98	ADV	063	42	STO	103	73	RC*
024	87	IFF	064	54	54	104	52	52
025	01	01	065	76	LBL	105	95	=
026	38	SIN	066	30	TAN	106	44	SUM
027	91	R/S	067	43	RCL	107	50	50
028	99	PRT	068	57	57	108	01	1
029	65	×	069	42	STO	109	32	X⇌T
030	02	2	070	53	53	110	43	RCL
031	55	÷	071	76	LBL	111	52	52
032	43	RCL	072	33	X^2	112	67	EQ
033	59	59	073	75	-	113	24	CE
034	95	=	074	01	1	114	02	2
035	42	STO	075	95	=	115	22	INV
036	47	47	076	42	STO	116	44	SUM
037	91	R/S	077	52	52	117	53	53
038	99	PRT	078	53	(	118	43	RCL
039	85	+	079	43	RCL	119	53	53

(Continued next page)

(Continued) Table II

Step	Key	Code	Step	Key	Code	Step	Key	Code
120	61	GTO	158	01	1	196	61	GTO
121	33	X^2	159	32	X:T	197	30	TAN
122	76	LBL	160	43	RCL	198	76	LBL
123	24	CE	161	50	50	199	23	LNX
124	87	IFF	162	75	-	200	53	(
125	01	01	163	43	RCL	201	43	RCL
126	45	Y^X	164	58	58	202	56	56
127	43	RCL	165	95	=	203	85	+
128	55	55	166	42	STO	204	43	RCL
129	65	×	167	49	49	205	55	55
130	43	RCL	168	50	IXI	206	54	)
131	46	46	169	22	INV	207	55	÷
132	95	=	170	77	GE	208	02	2
133	42	STO	171	39	COS	209	95	=
134	45	45	172	00	0	210	48	EXC
135	33	X^2	173	32	X:T	211	55	55
136	35	1/X	174	43	RCL	212	42	STO
137	65	×	175	49	49	213	54	54
138	53	(	176	22	INV	214	00	0
139	43	RCL	177	77	GE	215	42	STO
140	45	45	178	23	LNX	216	50	50
141	85	+	179	53	(	217	61	GTO
142	24	CE	180	43	RCL	218	30	TAN
143	94	+/-	181	55	55	219	76	LBL
144	22	INV	182	85	+	220	39	COS
145	23	LNX	183	43	RCL	221	43	RCL
146	75	-	184	54	54	222	55	55
147	01	1	185	54	)	223	65	×
148	54	)	186	55	÷	224	01	1
149	65	×	187	02	2	225	00	0
150	43	RCL	188	95	=	226	00	0
151	47	47	189	48	EXC	227	95	=
152	95	=	190	55	55	228	58	FIX
153	44	SUM	191	42	STO	229	01	01
154	50	50	192	56	56	230	99	PRT
155	76	LBL	193	00	0	231	98	ADV
156	45	Y^X	194	42	STO	232	91	R/S
157	93	.	195	50	50			

User instructions for DCFRR programs **Table III**

Step	Enter	Press	Display C*	Display D*	Print
1	C_0, Net initial investment	A	C_0	C_0	C_0
2	n, Economic life	R/S	C_0/n	n	n
3	N, No. cash-flow components†	R/S	$2N$	$2N$	N
4	IR_T, Investment × tax rate**	R/S	$2IR_T/n$	$2IR_T$	IR_T
5	T, Depreciable life	R/S	$T+0.5$	$T+0.5$	T
6	i_1, First cost-escalation rate‡	R/S	i_1	i_1	i_1
7	C_1, First cash-flow component	R/S	C_1	C_1	C_1
8	i_2, Second cost-escalation rate‡	R/S	i_2	i_2	i_2
9	C_2, Second cash-flow component	R/S	C_2	C_2	C_2
2N+4	i_N, Final cost-escalation rate‡	R/S	i_N	i_N	i_N
2N+5	C_N, Final cash-flow component	R/S	–	–	C_N
2N+6	Calculates DCFRR in percent	–	DCFRR	DCFRR	DCFRR

Notes:

* C: Continuous program; D: Discrete program
† Maximum N=22
** Omit steps 4 and 5 with Flag 1 set (before-tax mode)
‡ Enter i values as decimals (use zeros as applicable)

The number of pairs of cash flow components and corresponding escalation rates is limited to 22 by the availability of storage registers. However, this quantity should be ample for almost any analysis.

The first trial in the program uses a 25% discount rate. The program is limited to DCFRR values between 0% and 50%. If the calculation seems to be taking too long (i.e., 3 or 4 min), the DCFRR may be beyond these limits. This can be checked by stopping the program and exchanging the display with the contents of Register **55** (which contains the current discount rate). If the value is high (above 0.499) or low (below 0.001), the limits may have been exceeded. This can be further checked by again exchanging the display and Register **55**, then the display and Register **49**. An absolute value in Register **49** substantially above 0.1 gives stronger evidence that the DCFRR limits have been exceeded.

To extend the DCFRR limits of the continuous program, apply the following instructions (corresponding instructions for the discrete program appear in parentheses), after the direction of extension (higher or lower) has been indicated by the checking procedure.

To raise the DCFRR limit, enter the program at Location 061 (056), and replace the value of 0.5 that is stored in Register **54** with the desired higher limit (0.7, for example). Although it is unlikely that a negative DCFRR would be acceptable, the zero limit can also be extended by entering the program at Location 061 (056) and inserting the desired negative limit (−0.2, for example), then the instruction "Store 56." After extending the limits, rerun the entire program.

Note that the comparison basis for testing whether the DCFRR has been reached (NPV close to zero) is the value of 0.1 in locations 157 and 158 (161 and 162). This has been found sufficiently precise for the one decimal place (0.1%) to which DCFRR is carried out in the program. If this precision is greater than needed, the 0.1 test limit can be raised to shorten calculation time.

Continuous compounding is used for the depreciation discount factor in both the continuous and discrete programs. Discrete compounding for depreciation would require a loop that would add about 40 program steps and lengthen calculation time 15 s/iteration. This could add as much as 4 min to the discrete program, which already takes more time than the continuous one. The NPV difference between continuous and discrete compounding for depreciation is about 1½% of initial investment, which is ordinarily more precise than warranted by input data.

Although both programs are based on SOYD depreciation, they can be used without appreciable error for twice-straight-line depreciation. The NPV difference is usually less than 1% of the initial investment.

The programs do not include a provision for salvage value. It should be recalled that a cash flow from salvage does not occur until the property is disposed of at the end of its economic life, when the discount factor is usually quite low.

For HP-67/97 users

The HP version of the program has two parts, program A and program B; for listings, see Tables IV and V. Tables VI and VII contain user instructions for these programs.

Listing for HP version—program A for discrete compounding **Table IV**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	034	*LBL8	21 08	066	+	-55	098	RCL6	36 06	130	2	02
002	CLRG	16-53	035	+	-55	067	RCLA	36 11	099	CHS	-22	131	÷	-24
003	P⇄S	16-51	036	STO i	35 45	068	CHS	-22	100	e^x	33	132	STO9	35 09
004	CLRG	16-53	037	DSZI	16 25 46	069	e^x	33	101	RCL9	36 09	133	0	00
005	DSP2	-63 02	038	GTO1	22 01	070	CHS	-22	102	+	-55	134	STOE	35 15
006	STOI	35 46	039	RCL0	36 00	071	1	01	103	1	01	135	P⇄S	16-51
007	STO0	35 00	040	STOI	35 46	072	+	-55	104	-	-45	136	RCL0	36 00
008	R↓	-31	041	*LBL2	21 02	073	RCL8	36 08	105	x	-35	137	STOI	35 46
009	STOA	35 11	042	1	01	074	÷	-24	106	RCLD	36 14	138	GTO2	22 02
010	R↓	-31	043	RCL i	36 45	075	P⇄S	16-51	107	x	-35	139	*LBL5	21 05
011	STOB	35 12	044	FRC	16 44	076	RCL i	36 45	108	RCLE	36 15	140	RCL9	36 09
012	P⇄S	16-51	045	X>0?	16-44	077	INT	16 34	109	+	-55	141	STO7	35 07
013	.	-62	046	GTO9	22 09	078	X>0?	16-44	110	STOE	35 15	142	RCL6	36 06
014	2	02	047	1	01	079	GTO9	22 09	111	*LBL3	21 03	143	+	-55
015	5	05	048	+	-55	080	1	01	112	.	-62	144	2	02
016	STO9	35 09	049	*LBL9	21 09	081	-	-45	113	1	01	145	÷	-24
017	.	-62	050	+	-55	082	*LBL9	21 09	114	RCLE	36 15	146	STO9	35 09
018	5	05	051	RCL i	36 45	083	x	-35	115	RCLB	36 12	147	0	00
019	STO7	35 07	052	FRC	16 44	084	RCLE	36 15	116	-	-45	148	STOE	35 15
020	P⇄S	16-51	053	X>0?	16-44	085	+	-55	117	ABS	16 31	149	P⇄S	16-51
021	R/S	51	054	GTO9	22 09	086	STOE	35 15	118	X⇄Y	-41	150	RCL0	36 00
022	F1?	16 23 01	055	1	01	087	DSZI	16 25 46	119	X>Y?	16-34	151	STOI	35 46
023	GTO8	22 08	056	+	-55	088	GTO2	22 02	120	GTO4	22 04	152	GTO2	22 02
024	.	-62	057	*LBL9	21 09	089	P⇄S	16-51	121	RCLE	36 15	153	*LBL4	21 04
025	5	05	058	CHS	-22	090	F1?	16 23 01	122	RCLB	36 12	154	RCL9	36 09
026	+	-55	059	P⇄S	16-51	091	STO3	35 03	123	-	-45	155	1	01
027	STOC	35 13	060	RCL9	36 09	092	RCL9	36 09	124	X<0?	16-45	156	0	00
028	R↓	-31	061	+	-55	093	RCLC	36 13	125	GTO5	22 05	157	0	00
029	2	02	062	÷	-24	094	x	-35	126	RCL9	36 09	158	x	-35
030	x	-35	063	1/X	52	095	STO8	35 08	127	STO6	35 06	159	PRTX	-14
031	STOD	35 14	064	STO8	35 08	096	x^2	53	128	RCL7	36 07	160	SPC	16-11
032	*LBL1	21 01	065	1	01	097	1/X	52	129	+	-55	161	CF1	16 22 01
033	R/S	51										162	R/S	51

Listing for HP version—program B for continuous compounding **Table V**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	032	STOI	35 46	063	x	-35	094	x	-35	125	STOI	35 46
002	CLRG	16-53	033	P⇄S	16-51	064	P⇄S	16-51	095	RCLD	36 14	126	GTO2	22 02
003	P⇄S	16-51	034	.	-62	065	RCL i	36 45	096	x	-35	127	*LBL5	21 05
004	CLRG	16-53	035	2	02	066	P⇄S	16-51	097	RCLE	36 15	128	RCL9	36 09
005	DSP2	-63 02	036	5	05	067	INT	16 34	098	+	-55	129	STO8	35 08
006	STO0	35 00	037	STO9	35 09	068	X>0?	16-44	099	STOE	35 15	130	RCL6	36 06
007	STOI	35 46	038	.	-62	069	GTO9	22 09	100	*LBL3	21 03	131	+	-55
008	R↓	-31	039	5	05	070	1	01	101	RCLE	36 15	132	2	02
009	STOA	35 11	040	STO8	35 08	071	-	-45	102	RCLB	36 12	133	÷	-24
010	÷	-24	041	*LBL2	21 02	072	*LBL9	21 09	103	-	-45	134	STO9	35 09
011	STOB	35 12	042	RCL9	36 09	073	x	-35	104	STO7	35 07	135	0	00
012	F1?	16 23 01	043	P⇄S	16-51	074	RCLE	36 15	105	ABS	16 31	136	STOE	35 15
013	GTO1	22 01	044	RCL i	36 45	075	+	-55	106	.	-62	137	P⇄S	16-51
014	R/S	51	045	P⇄S	16-51	076	STOE	35 15	107	1	01	138	RCL0	36 00
015	.	-62	046	FRC	16 44	077	DSZI	16 25 46	108	X>Y?	16-34	139	STOI	35 46
016	5	05	047	X>0?	16-44	078	GTO2	22 02	109	GTO4	22 04	140	P⇄S	16-51
017	+	-55	048	GTO9	22 09	079	F1?	16 23 01	110	RCL7	36 07	141	GTO2	22 02
018	STOC	35 13	049	1	01	080	GTO3	22 03	111	X<0?	16-45	142	*LBL4	21 04
019	R↓	-31	050	+	-55	081	RCL9	36 09	112	GTO5	22 05	143	RCL9	36 09
020	2	02	051	*LBL9	21 09	082	RCLC	36 13	113	RCL9	36 09	144	1	01
021	x	-35	052	-	-45	083	x	-35	114	STO6	35 06	145	0	00
022	RCLA	36 11	053	RCLA	36 11	084	STO7	35 07	115	RCL8	36 08	146	0	00
023	÷	-24	054	x	-35	085	x^2	53	116	+	-55	147	x	-35
024	STOD	35 14	055	STO7	35 07	086	1/X	52	117	2	02	148	PRTX	-14
025	*LBL1	21 01	056	1/X	52	087	RCL7	36 07	118	÷	-24	149	CF1	16 22 01
026	R/S	51	057	RCL7	36 07	088	CHS	-22	119	STO9	35 09	150	SPC	16-11
027	+	-55	058	CHS	-22	089	e^x	33	120	0	00	151	R/S	51
028	STO i	35 45	059	e^x	33	090	RCL7	36 07	121	STOE	35 15			
029	DSZI	16 25 46	060	CHS	-22	091	+	-55	122	P⇄S	16-51			
030	GTO1	22 01	061	1	01	092	1	01	123	RCL0	36 00			
031	RCL0	36 00	062	+	-55	093	-	-45	124	P⇄S	16-51			

User instructions for HP version—program A for discrete compounding **Table VI**

	Key
For before-tax mode, set flag 1 **(STF 1)** before entering any data. For after-tax mode, run without any flags.	
Enter C_0, net initial investment	**ENTER ↑**
Enter *n*, economic life, yr	**ENTER ↑**
Enter *N*, number of cash flow components (maximum, 16)	key **A**
For after-tax mode (no flags set), enter the following data (for before-tax mode (flag 1 set), omit these data):	
Enter IR_T, Investment × tax rate	**ENTER ↑**
Enter T, depreciable life, yr	key **R/S**
For both tax modes:	
Enter cash flow components:	
Cost escalation rate *i*, decimal	**ENTER ↑**
Cost *C*, only dollars (no cents)	key **R/S**
(Enter *N* pairs of these items)	

When all data have been entered, program will automatically start calculating and output will be the discounted cash flow rate of return (DCFRR), in percent.

User instructions for HP version—program B for continuous compounding **Table VII**

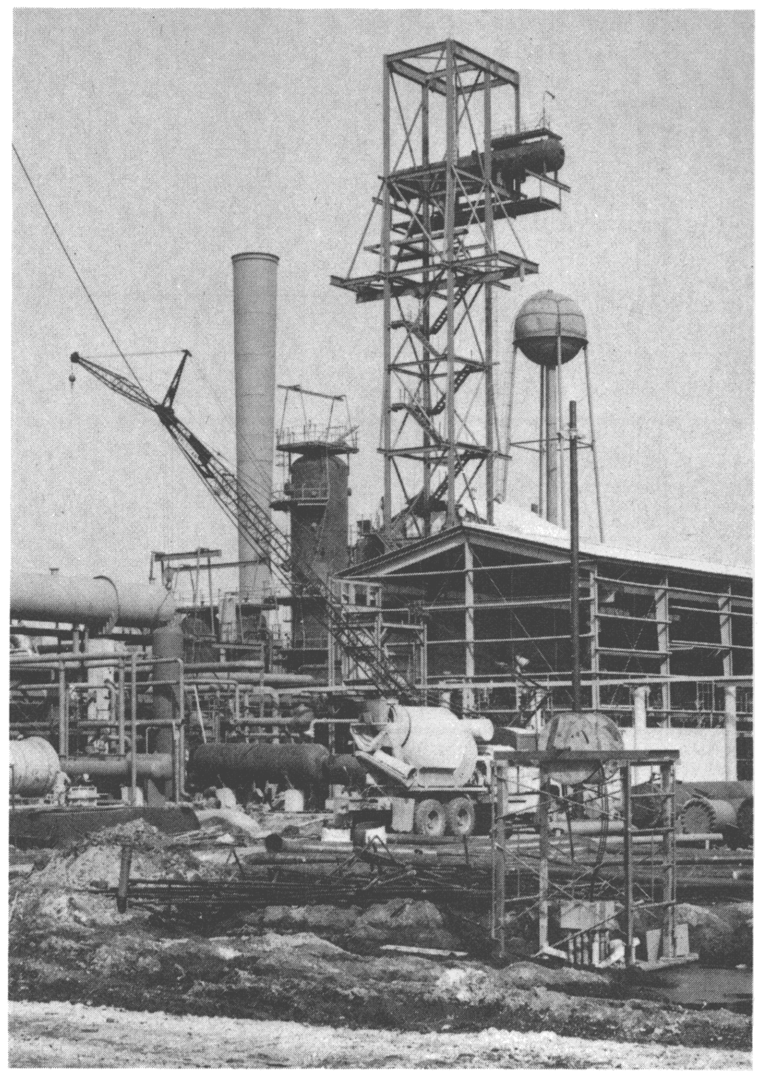
	Key
For before-tax mode, set flag 1 **(STF 1)** before entering any data. For after-tax mode, run without any flags.	
Enter C_0, net initial investment	**ENTER ↑**
Enter *n*, economic life, yr	**ENTER ↑**
Enter *N*, number of cash flow components (maximum, 16)	key **A**
For after-tax mode (no flags set), enter the following data (for before-tax mode (flag 1 set), omit these data):	
Enter IR_T, Investment × tax rate	**ENTER ↑**
Enter T, depreciable life, yr	key **R/S**
For both tax modes:	
Enter cash flow components:	
Cost escalation rate *i*, decimal	**ENTER ↑**
Cost *C*, only dollars (no cents)	key **R/S**
(Enter *N* pairs of these items)	

When all data have been entered, program will automatically start calculating and output will be the discounted cash flow rate of return (DCFRR), in percent.

Calculating net present value for varying cash flows

Knowing how project economics may change with varying underlying conditions can improve investment decisions. This program provides a tool for making analyses covering a range of possibilities.

Gordon W. Neal, Pacific Energy Consultants, Inc.



☐ Uncertainty in economic evaluations can be reduced by examining alternative projects under many likely conditions. This was shown in the article "Evaluating uncertainty in capital cost projections," *Chem. Eng.,* Sept. 6, 1982, p. 131.

Such comprehensive analyses are possible because of the availability of the programmable calculator and the computer. With the calculator, for instance, many scenarios can be investigated, rather than having an evaluation limited to only one set of conditions.

As was also discussed in the earlier article, there are two generally accepted bases for judging the economic attractiveness of projects: How much money will be generated, and how efficiently will the committed capital be used? A measure of the first is net present value (NPV), and of the second is discounted-cash-flow rate of return (DCFRR).

The program of Table I (for the TI-59 calculator) determines the NPV of an initial investment that is followed by a series of annual cash flows consisting of several components, each increasing or decreasing at a constant annual rate. It includes options for continuous or discrete compounding, and for after-tax or before-tax (e.g., government-funded) modes. The after-tax mode is based on sum-of-years-digits (SOYD) depreciation.

Originally published November 1, 1982.

Program calculates investment NPV for increasing or decreasing cash flows — **Table I**

Step	Code	Key	Step	Code	Key	Step	Code	Key	Step	Code	Key
000	76	LBL	035	99	PRT	070	57	57	133	85	+
001	11	A	036	85	+	071	54	)	134	24	CE
002	58	FIX	037	93	.	072	65	×	135	94	+/-
003	09	09	038	05	5	073	43	RCL	136	22	INV
004	47	CMS	039	95	=	074	58	58	137	23	LNX
005	99	PRT	040	42	STO	075	95	=	138	75	-
006	94	+/-	041	54	54	076	42	STO	139	01	1
007	42	STO	042	98	ADV	077	52	52	140	54	)
008	59	59	043	76	LBL	078	35	1/X	141	65	×
009	91	R/S	044	38	SIN	079	65	×	142	43	RCL
010	99	PRT	045	91	R/S	080	53	(	143	55	55
011	42	STO	046	99	PRT	081	01	1	144	95	=
012	58	58	047	72	ST*	082	75	-	145	44	SUM
013	91	R/S	048	00	00	083	43	RCL	146	59	59
014	99	PRT	049	97	DSZ	084	52	52	147	76	LBL
015	65	×	050	00	00	085	94	+/-	148	45	Y^X
016	02	2	051	38	SIN	086	22	INV	149	43	RCL
017	95	=	052	98	ADV	087	23	LNX	150	59	59
018	42	STO	053	76	LBL	088	54	)	151	58	FIX
019	57	57	054	33	X^2	089	65	×	152	01	01
020	42	STO	055	43	RCL	090	73	RC*	153	95	=
021	00	00	056	57	57	091	53	53	154	99	PRT
022	91	R/S	057	75	-	092	65	×	155	91	R/S
023	99	PRT	058	01	1	093	43	RCL	156	76	LBL
024	42	STO	059	95	=	094	58	58	157	44	SUM
025	56	56	060	42	STO	095	95	=	158	43	RCL
026	98	ADV	061	53	53	096	76	LBL	159	56	56
027	87	IFF	062	87	IFF	097	34	√X	160	75	-
028	01	01	063	02	02	098	44	SUM	161	73	RC*
029	38	SIN	064	44	SUM	099	59	59	162	57	57
030	91	R/S	065	53	(	100	01	1	163	95	=
031	99	PRT	066	43	RCL	101	32	X:T	164	55	÷
032	42	STO	067	56	56	102	43	RCL	165	53	(
033	55	55	068	75	-	103	53	53	166	01	1
034	91	R/S	069	73	RC*	104	67	EQ	167	85	+
						105	24	CE	168	73	RC*
						106	02	2	169	57	57
						107	22	INV	170	54	)
						108	44	SUM	171	95	=
						109	57	57	172	42	STO
						110	61	GTO	173	52	52
						111	33	X^2	174	35	1/X
						112	76	LBL	175	65	×
						113	24	CE	176	53	(
						114	87	IFF	177	01	1
						115	01	01	178	75	-
						116	45	Y^X	179	53	(
						117	43	RCL	180	01	1
						118	56	56	181	85	+
						119	65	×	182	43	RCL
						120	43	RCL	183	52	52
						121	54	54	184	54	)
						122	95	=	185	45	Y^X
						123	42	STO	186	43	RCL
						124	51	51	187	58	58
						125	33	X^2	188	94	+/-
						126	35	1/X	189	54	)
						127	65	×	190	65	×
						128	02	2	191	73	RC*
						129	65	×	192	53	53
						130	53	(	193	95	=
						131	43	RCL	194	61	GTO
						132	51	51	195	34	√X

User instructions for NPV program — **Table II**

Set desired flags:

Flag 1 – Before-tax mode

Flag 2 – Discrete compounding

Step	Enter	Press	Display	Print
1	C_0, net initial investment	A	$-C_0$	C_0
2	n, Economic life	R/S	n	n
3	N, Number of cash-flow components*	R/S	$2N$	N
4	R, Discount rate†	R/S	R	R
5	IR_T, Investment × tax rate‡	R/S	IR_T	IR_T
6	T, Depreciable life‡	R/S	T+0.5	T
7	i_1, First cost-escalation rate†	R/S	i_1	i_1
8	C_1, First cash-flow component	R/S	C_1	C_1
9	i_2, Second cost-escalation rate†	R/S	i_2	i_2
10	C_2, Second cash-flow component	R/S	C_2	C_2
$2N$+5	i_N, Final cost-escalation rate†	R/S	i_N	i_N
$2N$+6	C_N, Final cash-flow component	R/S		C_N
$2N$+7	Calculates NPV		NPV	NPV

*Maximum N = 25

†Enter R and i values as decimals (using zeros as applicable).

‡Omit steps 5 and 6 with Flag 1 set (before-tax mode).

Calculated NPV values at 50% tax rate and credits of 20% **Table III**

Input	Output: Example 1 – continuous compounding, after-tax mode (no flags)	Example 2 – discrete compounding, after-tax mode (Flag 2)	Example 3 – continuous compounding, before-tax mode (Flag 1)
C_0	522.	522.	652.
n	20.	20.	20.
N	4.	4.	4.
R	0.1	0.1	0.1
IR_T	326.	326.	
T	11.	11.	
i_1	0.09	0.09	0.09
C_1	122.	122.	244.
i_2	0.09	0.09	0.09
C_2	-45.	-45.	-90.
i_3	0.12	0.12	0.12
C_3	-13.	-13.	-26.
i_4	0.05	0.05	0.05
C_4	-19.	-19.	-38.
NPV	543.9	551.7	1019.8

Program formulas

The general formula used in the program is:

$$\text{NPV} = (C_1D_1 + C_2D_2 + \ldots + C_ND_N) + IR_TD - C_0 \quad (1)$$

Here, NPV = net present value, in any monetary unit; C_1, $C_2 \ldots C_N$ = first-year cash-flow components; D_1, $D_2 \ldots D_N$ = discount factor corresponding to cash-flow component with the same subscript; I = total investment; R_T = income tax rate; D = depreciation discount factor; and C_0 = net initial investment.

Equations for cash-flow-component discount factors are:

$$D_c = (1 - e^{-rn})/r \quad (2)$$

$$D_d = [1 - (1 + r)^{-n}]r \quad (3)$$

Here, D_c, D_d = discount factors for, respectively, continuous and discrete compounding; r = effective discount rate; and n = project's economic life, yr.

Expressions for, respectively, continuous and discrete effective discount rates are:

$$r_c = R - i \quad (4)$$

$$r_d = (R - i)/(1 + i) \quad (5)$$

Here, R = selected discount rate, and i = annual rate at which cash-flow component increases (use negative sign for decreasing rate).

The equation for the depreciation discount factor, based on continuous compounding and SOYD depreciation is:

$$D = 2\,(RT' + e^{-RT'} - 1)/(RT')^2 \quad (6)$$

Here, $T' = T + 1/2$, and T = depreciable life, yr.

Preparing and entering data

User instructions are in Table II. Note that the data-entering sequence is altered by the tax mode selected.

In the after-tax mode, the initial investment (C_0) should be adjusted to reflect any such items as investment and energy tax credits. Also, first-year cash-flow components, C_1, C_2, etc., are multiplied by $(1 - R_T)$ to arrive at the input values. In the before-tax mode, the full initial investment is used, and the first-year cash-flow components are not adjusted.

Depreciation is used only in the after-tax mode. The term $(I\ R_T)$ represents the full initial investment without credits multiplied by the tax rate.

Components of cash flow into the project (receipts, reduced costs) have positive signs, and those flowing out (expenses, increased costs) have negative signs.

Program features

Flags are set by the user to determine the compounding method and tax mode. When no flags are set, the program uses continuous compounding and the after-tax mode. Setting Flag 1 places the program in the before-tax mode. Setting Flag 2 prepares the program for discrete compounding. With both flags set, the program operates in the after-tax mode with discrete compounding.

The number of pairs of cash-flow components and corresponding escalation rates is limited to 25 by the availability of storage registers. This should be ample for almost any case.

Continuous compounding is used for the depreciation discount factor under both the continuous and discrete options. Although program steps could be added to accomplish discrete compounding for depreciation, this would require another loop of about 70 additional steps. The NPV difference between continuous and discrete compounding is normally about 1½% of the initial investment. Greater precision is usually not warranted by the input data.

Although the program is based on SOYD depreciation, it can be used for twice-straight-line depreciation without appreciable error. The NPV difference between the two methods is ordinarily something less than 1% of the initial investment.

Also, the program does not provide for salvage value. This can be accounted for by adding to NPV the product of the salvage value and the discount factor for the last year of economic life.

Calculation time varies with the number of cash-flow components. It runs about two seconds plus three seconds per cash-flow component (i.e., 11 s for three components, 14 s for four). Changes in compounding method or tax mode do not appreciably affect calculation time.

Examples of printouts are shown in Table III. Note that all of the examples are based on the same data, with an income tax rate of 50% and a combined investment and energy tax credit of 20%.

For HP-67/97 users

A listing of the HP version is shown in Table IV. User instructions are listed in Table V.

Program listing for HP version **Table IV**

Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code	Step	Key	Code
001	*LBLA	21 11	030	*LBL2	21 02	059	GTO9	22 09	088	RCLE	36 15	117	+	-55
002	STOA	35 11	031	F0?	16 23 00	060	1	01	089	×	-35	118	×	-35
003	R↓	-31	032	GTO4	22 04	061	-	-45	090	RCLC	36 13	119	P⇄S	16-51
004	STOI	35 46	033	RCLA	36 11	062	*LBL9	21 09	091	+	-55	120	STO9	35 09
005	STO0	35 00	034	RCLi	36 45	063	×	-35	092	STOC	35 13	121	1/X	52
006	R↓	-31	035	FRC	16 44	064	*LBLB	21 12	093	PRTX	-14	122	RCL9	36 09
007	STOB	35 12	036	X>0?	16-44	065	RCLC	36 13	094	CF0	16 22 00	123	1	01
008	R↓	-31	037	GTO9	22 09	066	+	-55	095	R/S	51	124	P⇄S	16-51
009	CHS	-22	038	1	01	067	STOC	35 13	096	*LBL3	21 03	125	+	-55
010	STOC	35 13	039	+	-55	068	DSZI	16 25 46	097	RCLC	36 13	126	RCLB	36 12
011	F1?	16 23 01	040	*LBL9	21 09	069	GTO2	22 02	098	PRTX	-14	127	CHS	-22
012	GTO1	22 01	041	-	-45	070	F1?	16 23 01	099	CF1	16 22 01	128	y^x	31
013	R/S	51	042	RCLB	36 12	071	GTO3	22 03	100	R/S	51	129	CHS	-22
014	STOD	35 14	043	×	-35	072	RCLA	36 11	101	*LBL4	21 04	130	1	01
015	R↓	-31	044	P⇄S	16-51	073	RCLD	36 14	102	RCLi	36 45	131	+	-55
016	STOE	35 15	045	STO9	35 09	074	×	-35	103	FRC	16 44	132	×	-35
017	RCLD	36 14	046	1/X	52	075	STOI	35 46	104	X>0?	16-44	133	RCLi	36 45
018	.	-62	047	1	01	076	X^2	53	105	GTO9	22 09	134	INT	16 34
019	5	05	048	RCL9	36 09	077	1/X	52	106	1	01	135	X>0?	16-44
020	+	-55	049	CHS	-22	078	2	02	107	+	-55	136	GTO9	22 09
021	STOD	35 14	050	e^x	33	079	×	-35	108	*LBL9	21 09	137	1	01
022	*LBL1	21 01	051	-	-45	080	RCLI	36 46	109	ENT↑	-21	138	-	-45
023	R/S	51	052	×	-35	081	CHS	-22	110	ENT↑	-21	139	*LBL9	21 09
024	+	-55	053	RCLB	36 12	082	e^x	33	111	1	01	140	×	-35
025	STOi	35 45	054	×	-35	083	RCLI	36 46	112	+	-55	141	GTOB	22 12
026	DSZI	16 25 46	055	P⇄S	16-51	084	+	-55	113	1/X	52	142	-	-45
027	GTO1	22 01	056	RCLi	36 45	085	1	01	114	X⇄Y	-41	143	R/S	51
028	RCL0	36 00	057	INT	16 34	086	-	-45	115	CHS	-22			
029	STOI	35 46	058	X>0?	16-44	087	×	-35	116	RCLA	36 11			

User instructions for HP version **Table V**

Case 1. For continuous compounding, after-tax mode. No flags.	
Case 2. For discrete compounding, after-tax mode. Set Flag 0	**STF 0**
Case 3. For condinuous compounding, before-tax mode. Set Flag 1	**STF 1**
All cases:	
Enter C_0, net initial investment	**ENTER ↑**
Enter n, economic life, yr	**ENTER ↑**
Enter N, number of cash flow components (maximum, 18)	**ENTER ↑**
Enter R, discount rate, in decimal form	key **A**
For cases 1 and 2 (Omit this input with case 3):	
Enter IR_T, investment × tax rate	**ENTER ↑**
Enter T, depreciable life, yr	key **R/S**
For all cases:	
Enter cash flow components:	
Cost escalation rate i, decimal	**ENTER ↑**
Cost C, dollars only (no cents)	key **R/S**
(Enter N pairs of these items.)	

When all data have been entered, program will automatically start calculating and output will be the net present value (NPV).

The author

Gordon W. Neal founded Pacific Energy Consultants, Inc. (1000 Quail St., Suite 290, Newport Beach, CA 92660; telephone 714-955-0493), which deals with all stages of project development, with emphasis on energy conservation. The projects cover technical and economic feasibility analyses, design and construction coordination in the fields of cogeneration, heating, air conditioning, ventilation and refrigeration. A registered engineer in 11 states and a member of numerous professional associations, he holds a B.Sc. in mechanical engineering from the University of Nebraska.

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