NIST

NIST Standard Reference Database 23

NIST Reference Fluid Thermodynamic and Transport Properties—REFPROP

Version 7.0

Users' Guide

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1. INTRODUCTION

1.1 Objectives and Scope of the Database

REFPROP is an acronym for REference Fluid PROPerties. This program, developed by the National Institute of Standards and Technology (NIST) provides tables and plots of the thermodynamic and transport properties of industrially important fluids and their mixtures with an emphasis on refrigerants and hydrocarbons.

REFPROP is based on the most accurate pure fluid and mixture models currently available. It implements three models for the thermodynamic properties of pure fluids: equations of state explicit in Helmholtz energy, the modified Benedict-Webb-Rubin equation of state, and an extended corresponding states (ECS) model. Mixture calculations employ a model which applies mixing rules applied to the Helmholtz energy of the mixture components; it uses a departure function to account for the departure from ideal mixing. Viscosity and thermal conductivity are modeled with either fluid-specific correlations or an ECS method.

These models are implemented in a suite of FORTRAN subroutines. They are written in a structured format, are internally documented with extensive comments, and have been tested on a variety of compilers. Routines are provided to calculate thermodynamic and transport properties at a given (T,ρ,x) state. Iterative routines provide saturation properties, including surface tension, for a specified (T,x) or (P,x) state. Flash calculations describe single- or two-phase states given a wide variety of input combinations [(P,h,x), (P,T,x), etc].

A separate graphical user interface, designed for the Windows operating system, provides a convenient means of accessing the models. It generates tables and plots for a user-specified mixture or a number of predefined mixtures (air and the commercially available refrigerant blends). An on-line help system provides information on how to use the program. Information screens that display fluid constants and documentation for the property models can be called up at any time. Numerous options to customize the output are available as well as capabilities to copy and paste to and from other applications.

The property models can also be accessed by other applications (such as spreadsheets) through use of a provided dynamic link library (DLL).

1.2 Uncertainties in Calculated Properties

Our objective in selecting property models for use in REFPROP was to implement the most accurate models currently available. The user should be aware that the uncertainties in these models vary considerably depending on the fluid, property, and thermodynamic state. It is thus impossible to give a simple, global statement of uncertainties. Even for the most-studied fluids with equations of state based on accurate, wide-ranging data, uncertainties are complicated functions of the temperature and pressure. The interested user is referred to the original literature sources for details. (References to the literature are accessible through the fluid and mixture information screens described in Sections 4.4.1 and 4.5.)

The user is further cautioned that, by the very nature of a calculations database, property data are often displayed with more digits than can be justified based on the accuracy of the property models or the uncertainties in the experimental data to which the models were fitted.

1.3 Organization of the Users' Guide

Section 2 details the installation procedure. Section 3 presents a brief overview of the structure of the database and its main features. Sections 4 through 11 describe the features of the database in detail. The fluids in the database are tabulated in Appendix A. The property models used in the database and their sources are outlined in Appendix B. Use of the FORTRAN property subroutines is described in Appendix C. Use of the property routines with Excel spreadsheets and VisualBasic programs is outlined in Appendix D. Appendix E contains a reference listing of warnings and error messages generated by the property routines. Finally, Appendix F lists support contacts at NIST.

NOTE: The figures in this manual show windows and dialogs as they appear in the Windows® 98 operating environment. If you are in another environment, their appearance may be slightly different.

2. INSTALLATION

2.1 System Requirements

REFPROP is designed to run on any personal computer running the Microsoft® Windows® 3.1, 95, 98, 2000, or NT operating system. A Pentium® processor (or 486 with a math coprocessor) is required. The program requires 5.0 MB of hard disk space.

NOTE: Database may not run properly on Korean Window installations.

2.2 Installation

Place the REFPROP CD-ROM in the CD drive. In Windows NT™ version 3.51, Windows 9x, Windows 2000 4.0, Windows Me and Windows XP select the **File**

Click [**START**], select [**RUN**] type in: **M:\setup**

Follow the remainder of the Installation instructions.

3. OVERVIEW

This section presents a brief overview of the database and its main features. Please refer to the remaining sections in this Users' Guide for more complete information.

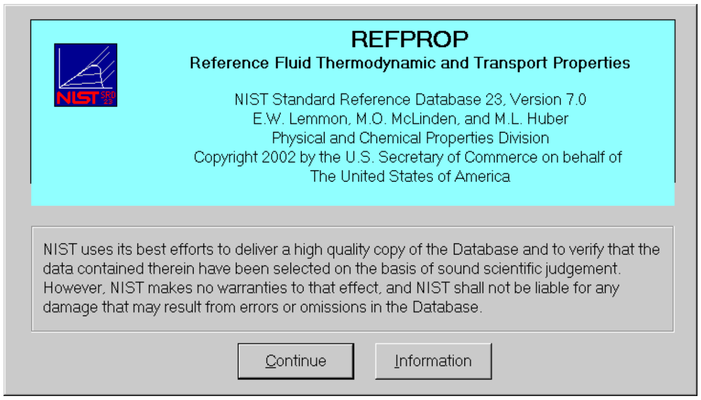
3.1 Database Structure

REFPROP consists of a graphical user interface (GUI) and subroutines implementing a variety of fluid property models. The interface provides a convenient means to calculate and display thermodynamic and transport properties of pure fluids and mixtures. The property models are written in FORTRAN and accessed by the GUI through a dynamic link library (DLL). The property subroutines can also be used independently of the GUI, as described in Appendix C. The DLL can also be utilized by other applications, such as spreadsheets, as described in Appendix D.

The high-level subroutines that carry out iterative saturation and flash calculations are independent of the fluid property models. Underlying these subroutines are sets of core routines for each of the models implemented in the database. The numerical coefficients to the property models for each fluid are stored in separate text files. The coefficients for the mixture departure functions are stored in a single text file. Additional files contain information specifying predefined or user-defined mixtures. This structure simplifies the addition of new fluids and additional models to future versions of the database and makes such additions almost totally transparent to the user.

3.2 Use of the Database

Start the REFPROP database by double-clicking on its icon. A banner screen displays the title, credits, and a legal disclaimer. Clicking the "Information" button calls up further details and credits through the on-line help system. Clicking the "Continue" button starts the database. The program is controlled, in the usual fashion of a Windows application, by the use of pull-down menus displayed across the top of the application window.



REFPROP

Reference Fluid Thermodynamic and Transport Properties

NIST Standard Reference Database 23, Version 7.0
E.W. Lemmon, M.O. McLinden, and M.L. Huber
Physical and Chemical Properties Division
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Start-up screen for the REFPROP database.

3.3 Overview of the Menus

The File menu provides commands to save and print generated tables and plots. Individual items or entire sessions with multiple windows can be saved or recalled. The standard Print, Print Setup, and Exit commands are also present.

The Edit menu provides copy and paste commands, which allow selected data or plots to be exchanged with other applications.

The Options menu provides commands for selecting the unit system, properties of interest, the reference state, and user preferences. These options can be stored for recall. A user-defined set of preferences is loaded upon program startup.

The pure fluid or mixture of interest is specified with commands in the Substance menu. Most refrigerant mixtures of current commercial interest (those having an ASHRAE R400- or R500-series designation) are predefined. Standard air is also predefined. In addition, new mixtures with up to 20 components can be specified and saved.

The Calculate menu initiates the calculations that generate a property table. Each property selected for display is shown in a separate column of the table. Two types of tables are provided.

The first provides properties either at saturation or with a property (such as density or enthalpy) held constant with temperature or pressure varying over a specified range. The second allows the user to select the independent variables. Values of the independent variables can be entered with the keyboard, read from a file, or pasted from another application.

The Plot menu provides x-y plots of properties appearing in a table. In addition, simple plots of the thermodynamic surface can be easily generated on a wide range of coordinates, including temperature-entropy and pressure-enthalpy. Temperature-composition, and pressure-composition diagrams for binary mixtures can be generated automatically. Commands are provided to modify the plot size, axis scaling, plot symbols, line type, legend, and other plot features.

Each table or plot appears in a separate window and can be accessed, resized, or retitled with commands in the Window menu. The number of windows is limited only by available memory.

A complete online-help system can be accessed through the Help menu.

A status line at the bottom of the screen displays the currently specified fluid or mixture, composition, and reference state. Clicking on the status line (or the Substance/Fluid Information command) calls up information screen(s) for the mixture and each of the components, thereby providing documentation for fluid constants, the source of the models, equation of state uncertainties, and their range of applicability.

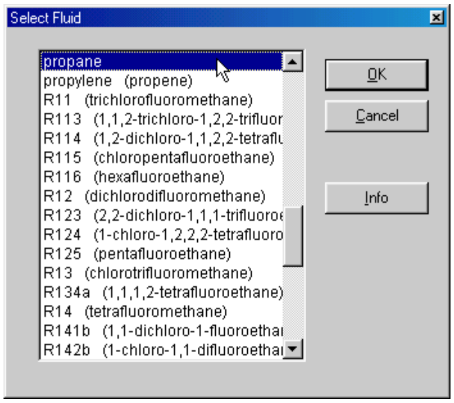
The menus and dialogs are typically navigated with the mouse. Keyboard shortcuts are also available for virtually all actions. These are activated by the “Alt” key in combination with the underlined letter of the individual command. The TAB key moves between items in a dialog.

4. DEFINING THE FLUID OF INTEREST
(The Substance Menu)

The Substance menu defines the fluid or mixture for subsequent properties calculations. Predefined mixtures can be selected or new mixtures of up to 20 components can be defined. Defining a new fluid or mixture has no effect on tables or plots already produced.

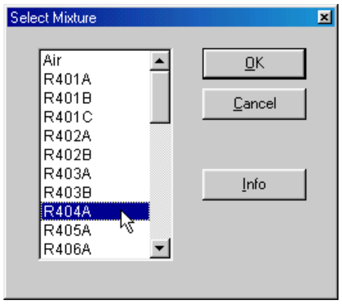
4.1 Selecting a Pure Fluid

Selecting the Pure Fluid item in the Substance menu brings up the dialog box shown below. The available fluids are shown in a scrollable list on the left. (The fluids available in the database are also tabulated in Appendix A.) Select the fluid you want to investigate by clicking the mouse button on the fluid name. You can jump quickly to a fluid by typing the beginning letter(s) of its name. Clicking on the Info button brings up an information screen of fluid constants (such as molecular weight and normal boiling point) and reference information. The information screen is described in more detail in Section 4.4.1. By clicking the OK button all subsequent property calculations are carried out on the selected fluid. The fluid name is displayed in the status bar at the bottom of the screen to confirm this choice. If you want to retain the previous fluid choice, click the Cancel button



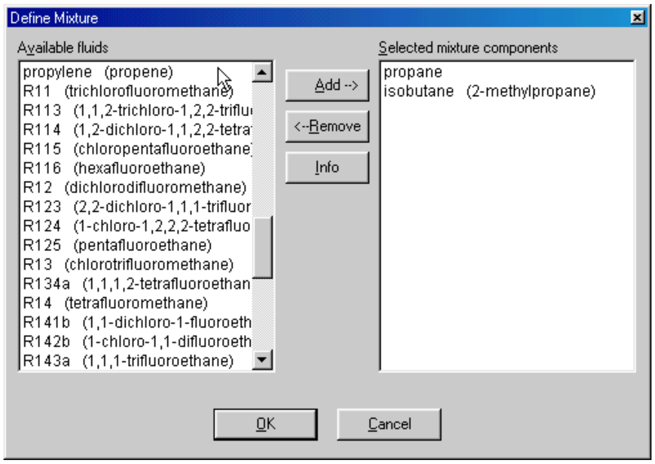
4.2 Selecting a Predefined Mixture

Predefined mixtures are specified in a way analogous to that for pure fluids by selecting the Predefined Mixture item in the Substance menu. The predefined mixtures include dry air and a number of commercially available refrigerant blends. Additional mixtures can be added to this dialog by saving a mixture in the Define New Mixture dialog described in Section 4.3. The one significant difference between the Pure Fluid and Predefined Mixture dialogs is the effect of the Info button. Clicking the Info button brings up a Mixture Information screen as described in Section 4.4.3.



4.3 Defining a New Mixture

The Define New Mixture item in the Substance menu brings up the dialog shown below and allows specification of a mixture of up to 20 components. Note that not all mixtures are allowed. The scrollable list on the left shows the available pure fluids. A mixture is composed by clicking on a fluid name to select it and then clicking the Add button (or simply double-click the fluid name) to add it to the list of mixture components on the right. To remove a component from the mixture, click its name to highlight it and click the Remove button (or simply double-click). Notice that when a fluid is added to the right list, it disappears from the list of available pure fluids on the left; this prevents inadvertently defining a mixture composed of two identical components. The pure fluid information screen for any component can be called up by selecting a fluid name and clicking the Info button.



Available fluids:

propylene (propene)
R11 (trichlorofluoromethane)
R113 (1,1,2-trichloro-1,2,2-triflu
R114 (1,2-dichloro-1,1,2,2-tetra
R115 (chloropentafluoroethane)
R116 (hexafluoroethane)
R12 (dichlorodifluoromethane)
R123 (2,2-dichloro-1,1,1-trifluor
R124 (1-chloro-1,2,2,2-tetrafluo
R125 (pentafluoroethane)
R13 (chlorotrifluoromethane)
R134a (1,1,1,2-tetrafluoroethan
R14 (tetrafluoromethane)
R141b (1,1-dichloro-1-fluoroeth
R142b (1-chloro-1,1-difluoroeth
R143a (1,1,1-trifluoroethane)

Selected mixture components:

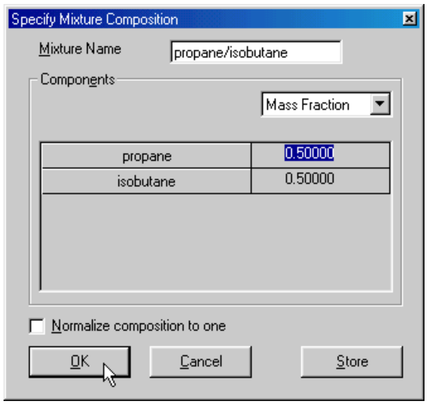
propane
isobutane (2-methylpropane)

In addition, multiple selections can be made by either holding down the Ctrl key while selecting multiple fluids, or by holding down the Shift key to mark all fluids between the currently marked fluid, and the following one. You can also use the arrow keys to select a fluid, and press Alt-A to add it. The period and '>' keys will also add a fluid. Removing the fluid can be done with either Alt-R, a comma, or '<'. Fluids can be highlighted by typing in the first few letters of their names, for example, typing 'pr' will select propane; to get propylene, type 'propy'.

4.3.1 Defining the Mixture Name and Composition

The Specify Composition dialog shown below serves two purposes. First, it provides a means of specifying the composition of a fluid system consisting of more than one component. The second function provides an opportunity to store the fluid system so that it can later be selected with the Predefined Mixture command (as described in Section 4.2).

Clicking the OK button in the Define Mixture dialog brings up the Specify Mixture Composition dialog. The name given to the mixture defaults to a concatenation of the component names; this can be changed by typing any desired name into the edit box at the top of the dialog. The mixture composition is entered by typing the desired values into the edit boxes next to the component names. The composition can be specified in terms of either mass or mole fractions. The basis for the composition (mass or molar) corresponds to the basis specified in the Units dialog (see Section 7.1). Composition in the other basis can be entered by clicking the pull-down arrow and selecting either Mass fraction or Mole fraction. Clicking the name of a component brings up the pure fluid information screen for that component.



Mixture Name: propane/isobutane

Mass Fraction

propane	0.50000
isobutane	0.50000

☐ Normalize composition to one

If the entered compositions do not sum to one, an Alert box is displayed. Clicking the NO button returns you to the Specify Mixture Composition dialog where you can correct the error. Alternately, the check box near the bottom of the screen directs the interface to “Normalize compositions to one.” This option is useful if, for example, a blend is based on a recipe stated in absolute quantities of the various components rather than mass or mole fractions.

4.3.2 Storing a Mixture For Future Use

The Store button in the Specify Mixture Composition dialog allows you to store a mixture for future use. Clicking this button brings up a standard Windows file dialog. A new file containing the data necessary to specify the current mixture is placed in the Mixtures subdirectory of the working REFPROP directory. This new mixture is then available for future calculations directly from the Predefined Mixture dialog. Note that the mixture is identified by its name, not the name of the file storing its specification data. You can store a mixture at a later time by calling up the Specify Composition dialog and going directly to the Store dialog. You can edit the filename or change its location, but the interface recognizes ONLY the files in the Mixtures subdirectory having a “.mix” file name extension.

4.4 The Status Bar

A status bar at the bottom of the main window displays information about the current settings:

the fluid or mixture name,

the components of a mixture,

the mixture composition (if applicable); if a mass basis has been selected (under the Units option) the composition is expressed in mass percentages, *e.g.* (50/50), in accordance with ASHRAE Standard 34; if a molar basis has been selected, the composition is expressed in mole fractions, *e.g.* (0.50/0.50), and

the reference state for enthalpy and entropy calculations (see Section 7.2).

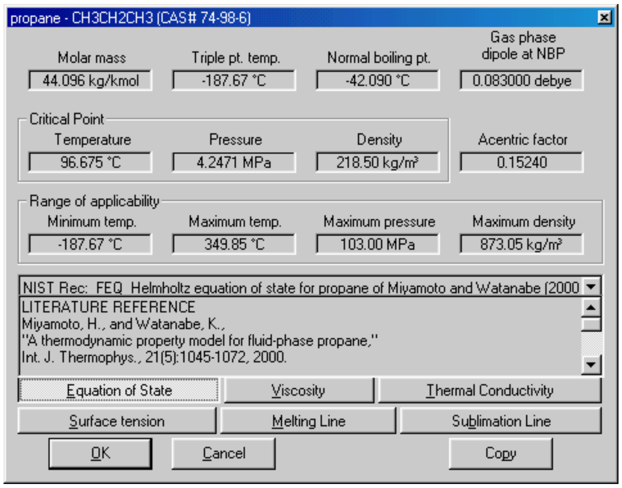
If the settings for the front most table or plot window displayed differ from the current settings, the information for that window is also displayed following the current settings information as shown below.

Current Fluid: R410A Components: R32/R125 (50/50) Current table: propane Ref. State: Default

Status bar showing current settings and a different set of settings which apply to the front window.

4.4.1 Pure-Fluid Information Screen

Clicking the status bar when a pure fluid is selected brings up an information screen. This screen is also displayed when a component name is clicked on the mixture information screen, the Specify New Mixture dialog, or the Specify Mixture Composition dialog. It can also be accessed through the Fluid Information command in the Substance menu.



propane - CH3CH2CH3 (CAS# 74-98-6)

Molar mass: 44.096 kg/kmol
Triple pt. temp.: -187.67 °C
Normal boiling pt.: -42.090 °C
Gas phase dipole at NBP: 0.083000 debye

Critical Point
Temperature: 96.675 °C
Pressure: 4.2471 MPa
Density: 218.50 kg/m³
Acentric factor: 0.15240

Range of applicability
Minimum temp.: -187.67 °C
Maximum temp.: 349.85 °C
Maximum pressure: 103.00 MPa
Maximum density: 873.05 kg/m³

NIST Rec: FEQ Helmholtz equation of state for propane of Miyamoto and Watanabe (2000

LITERATURE REFERENCE
Miyamoto, H., and Watanabe, K.,
"A thermodynamic property model for fluid-phase propane,"
Int. J. Thermophys., 21(5):1045-1072, 2000.

The top border of the screen gives the short name for the fluid, its full chemical name (if different from the short name), chemical formula, and its Chemical Abstracts Service (CAS) registry number. The top portion of the info screen displays fluid constants—the molar mass, the triple point and normal boiling point temperatures, the critical parameters, and the acentric factor. These are displayed in units corresponding to the current set as specified in the Units dialog (Section 7.1). Also displayed is the dipole moment; for those fluids with a temperature-dependent dipole moment, the value at the normal boiling point temperature is displayed. The number of digits displayed corresponds to that set in the preferences (Section 7.5)

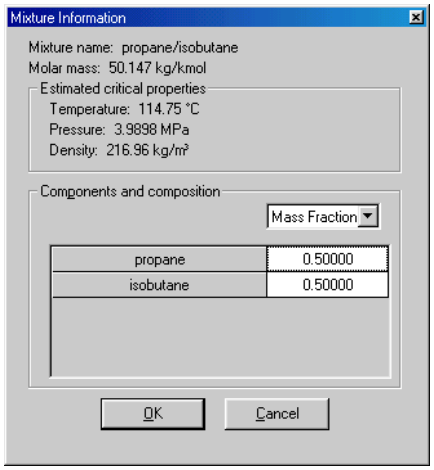
The bottom portion of the info screen provides information on the models used to calculate the various properties. Information on the equation of state and the viscosity, thermal conductivity, surface tension, melting line, and sublimation line models can be called up by clicking on the buttons near the bottom of the screen. (Note that melting and sublimation lines are not available for all fluids.) The "equation of state" refers to a property model used to calculate all of the thermodynamic properties, including density, vapor pressure, enthalpy, entropy, heat capacity, and speed of sound. The temperature, pressure, and density ranges over which the selected model is applicable are displayed near the middle of the screen. Below that a one-line description of the model is given. Finally, a literature reference, along with a statement of the uncertainties in the equation of state, is provided in a scroll box. The reference information can be copied to the Clipboard by highlighting the desired portions with the mouse and clicking the Copy button. Click the OK button to return to the previous window or dialog.

4.4.2 Changing property models

For some fluids, more than one model may be available for some of the properties. If multiple models are available, the list box arrow to the right of the one-line model description is active; click this arrow to display the available models. The recommended model is identified with the term "NIST rec." Additional (alternative) models are identified with the term "Alt. model." Select the model to be used in subsequent calculations by clicking on its name. This option should be used with caution. In most cases, the NIST-recommended model should be used. The main purpose of this option is to allow comparisons with models used in earlier versions of the NIST databases. Note that alternative models are not stored with other preferences (see Sections 7.6 and 8.1), so it would be necessary to specify an alternative model each time REFPROP is started.

4.4.3 Mixture Information Screen

Clicking the status bar when a mixture has been selected brings up the Mixture Information screen. This screen displays the name of the current mixture at the top of the screen. The estimated critical parameters and molecular weight for the specified composition are displayed. (The “estimated critical parameters” may differ from the true mixture critical parameters. The method used to calculate these parameters is discussed in Appendix B.) The components and their compositions are listed in the bottom part of the info screen. Clicking on a component name calls up the pure fluid info screen for that component. The basis for the composition (mass or molar) corresponds to the basis specified in the Units dialog. Composition in the other basis can be viewed by clicking the pull-down arrow and choosing either Mass fraction or Mole fraction. Clicking the OK button returns you to the underlying window or dialog.



Mixture name: propane/isobutane
Molar mass: 50.147 kg/kmol

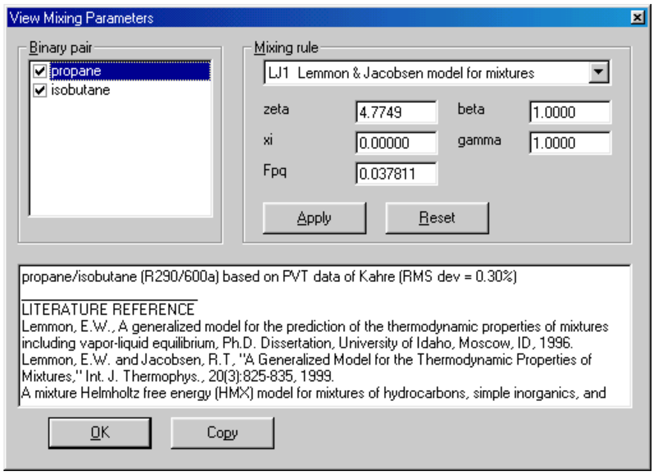
Estimated critical properties
Temperature: 114.75 °C
Pressure: 3.9898 MPa
Density: 216.96 kg/m³

Components and composition

propane	0.50000
isobutane	0.50000

4.5 Viewing Mixture Parameters

The View Mixing Parameters option displays the numerical values of the parameters used in calculating mixture thermodynamic properties and gives information on the data sources. This command is active only if a mixture is currently specified.



☑ propane
☑ isobutane

LJ1 Lemmon & Jacobsen model for mixtures

zeta 4.7749
beta 1.0000
xi 0.00000
gamma 1.0000
Fpq 0.037811

propane/isobutane (R290/600a) based on PVT data of Kahre (RMS dev = 0.30%)

LITERATURE REFERENCE
Lemmon, E.W., A generalized model for the prediction of the thermodynamic properties of mixtures including vapor-liquid equilibrium, Ph.D. Dissertation, University of Idaho, Moscow, ID, 1996.
Lemmon, E.W. and Jacobsen, R.T, "A Generalized Model for the Thermodynamic Properties of Mixtures," Int. J. Thermophys., 20(3):825-835, 1999.
A mixture Helmholtz free energy (HMX) model for mixtures of hydrocarbons, simple inorganics, and

The database calculates mixture properties by applying thermodynamic transformations to the Helmholtz energy. The mixture Helmholtz energy is calculated from the pure-fluid Helmholtz energies through the use of mixing rules. (See Appendix B for a description of the mixture model.) The mixing rules are applied to binary pairs of fluids, so for mixtures with three or more components the binary pair of interest must be specified by clicking the check boxes next to the component names. To view a different pair, click on the desired components.

The short-hand name of the mixing rule is displayed at the top right of the dialog. Below that are the numerical values for the parameters associated with that rule. The scroll box at the bottom of the dialog gives reference information. The top part of the box (above the line) gives a brief summary of the data used to determine the numerical coefficients. This information consists of a maximum of 255 characters because of limitations in passing information between the core property subroutines and the user interface. More complete information on the mixing rule can be obtained in the literature reference given in the bottom half of the scroll box. The reference information can be copied to the Clipboard by highlighting the desired portions with the mouse and clicking the Copy button. Click the Exit button to return to the main REFPROP window.

4.6 Changing Mixture Parameters

The View Mixing Parameters option also allows changing the numerical values of the mixture parameters used in calculating mixture thermodynamic properties. In some cases, it may be possible to improve the agreement between the calculated values and experimental data by altering these values. This command is not intended for the casual user, and great care must be used in altering these rules.

Select the binary pair of interest as described in Section 4.5. The recommended mixing rule is displayed at the upper right of the dialog. The numerical parameters for that rule are displayed below in edit boxes; type in new values for any you wish to change. Changes take effect only when the Apply button is clicked for a given binary pair. Each binary pair in a multicomponent mixture must be edited and “Applied” separately. (Note that when you click the Apply button the mixture-specific reference information in the bottom part of the screen is replaced by the message “Binary parameters for this binary pair have been modified from their original values.”)

It is also possible to change the mixing rule. The available mixing rules can be viewed by clicking on the drop-down arrow. An alternate rule can be chosen by clicking on it. When a different rule is chosen, the parameters associated with that rule are set to default values approximating ideal mixing. New values for these parameters can be entered as described above.

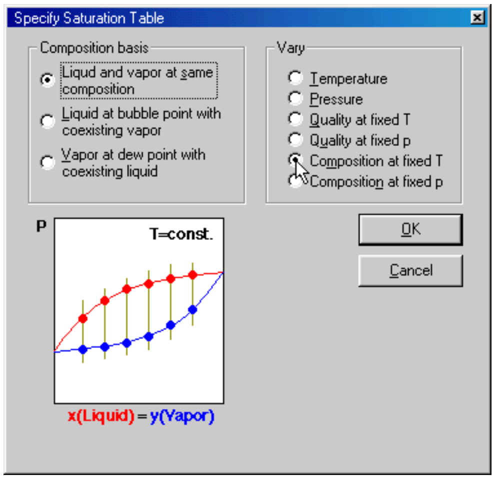
Clicking the OK button causes any changes made in the mixing rules or parameter values to be applied to all subsequent calculations. Clicking the Reset button resets all the mixing rules and their numerical parameters to the values originally read from the data file.

5. GENERATING PROPERTY TABLES (The Calculate Menu)

The Calculate menu provides several options for generating tables of two distinct types. The Saturation Tables and Iso-Property Tables options calculate properties at even spacings of temperature, pressure, density, composition, or quality at some fixed value of another property. The remaining options bring up spreadsheet-type windows which allow arbitrary values of the independent variables (including composition) to be entered in a variety of ways.

5.1 Calculating Saturation Tables

Selecting the Saturation Tables option in the Calculate menu brings up a dialog box from which the form of the table is specified. There are numerous options for saturation tables, especially for mixtures. Saturation tables display properties for the saturated liquid and saturated vapor, denoted by (Liquid Phase) and (Vapor Phase) in the table headings.



Specify Saturation Table

Composition basis

● Liqud and vapor at same composition
○ Liquid at bubble point with coexisting vapor
○ Vapor at dew point with coexisting liquid

Vary

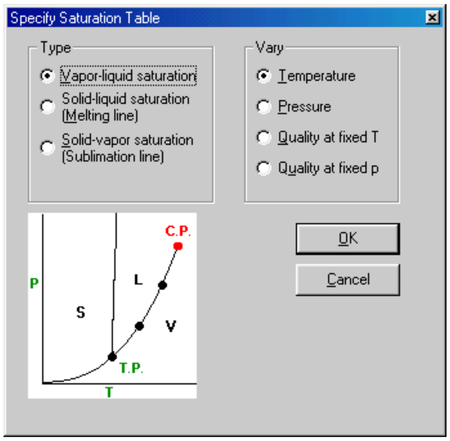
○ Temperature
○ Pressure
○ Quality at fixed T
○ Quality at fixed p
● Composition at fixed T
○ Composition at fixed p

The composition basis for the calculations is specified by the left set of radio buttons. The independent variable is specified by the right set of buttons. Choose one button from each list. A small phase diagram depicts the type of calculation to be performed; this diagram changes as different buttons in the two lists are chosen. The red and blue dots indicate the points to be calculated, and the gray lines connect liquid and vapor points that are displayed in a given row of a table.

Care should be excercised in selecting the desired composition basis. The liquid and vapor can be of the same composition, in which case the temperature or pressure of the liquid and vapor phases are not in equilibrium; this option is useful when working with a mixture of fixed composition. Alternately, the liquid and vapor can be in equilibrium with the specified composition set to either liquid at the bubble point or vapor at the dew point. In these cases, the temperature and pressure of the two phases are the same, but the compositions are different (except for the special case of an azeotrope).

Six choices are available for the property to be varied (right-hand set of radio buttons). The first four generate points at the composition of the mixture, the last two calculate properties at different compositions which have no connection to the composition specified when the system was set up.

For a pure fluid, not all the mixture choices are meaningful, and a simpler dialog is displayed. In addition to the normal vapor-liquid saturation, for some fluids solid-liquid saturation (melting line) and/or solid-vapor saturation (sublimation line) properties are available. These options are greyed out for those fluids lacking these data.

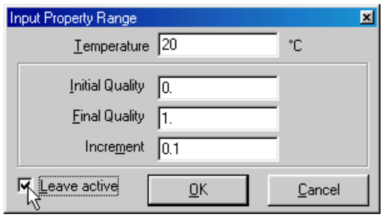


Specify Saturation Table

Type
- ● Vapor-liquid saturation
- ○ Solid-liquid saturation (Melting line)
- ○ Solid-vapor saturation (Sublimation line)

Vary
- ● Temperature
- ○ Pressure
- ○ Quality at fixed T
- ○ Quality at fixed p

From either the mixture or pure fluid dialog, clicking the OK button brings up a dialog in which the range and increment of the property to be varied and the value of the property to be held constant (if applicable) are entered. Default values are provided. The first time a table is calculated for a specific fluid, the defaults are based on the current units settings and the properties of the fluid or mixture. For subsequent calculations, the default values for the range and increment are those from the previous table. The range and increment revert to default values when a new fluid or mixture is specified. Deselecting the “Reset bounds...” option under Preferences retains the range and increment; see Section 7.5.



Temperature 20 °C

Initial Quality 0.

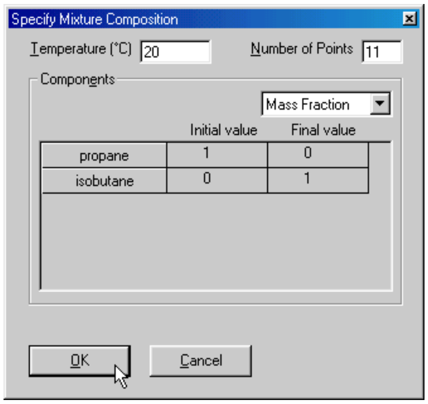
Final Quality 1.

Increment 0.1

☑ Leave active

The Leave active check box at the lower left keeps this dialog as the top window on the screen, allowing rapid calculation of a series of tables of the same type.

If the composition of the mixture is to be varied, the following window will appear:



Temperature (°C) 20

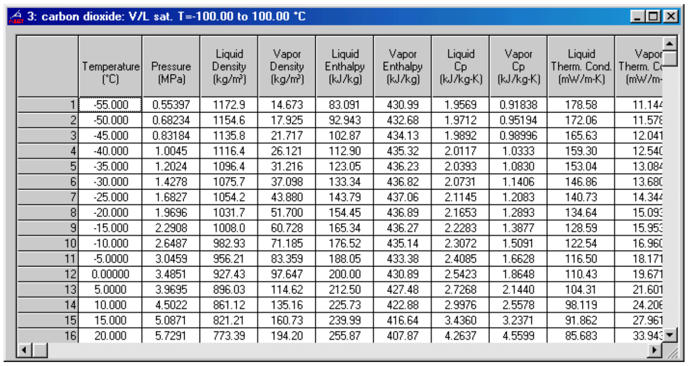
Number of Points 11

Mass Fraction

	Initial value	Final value
propane	1	0
isobutane	0	1

The constant property (temperature or pressure) is entered at the upper left. The composition will be linearly varied from the condition indicated in the "Initial" column to that in the "Final" column using the number of points indicated at the upper right. With 11 points, the composition of the binary system shown in the example is varied from pure component 1 to pure component 2 with increments of 0.1 in mass fraction.

Clicking the OK button initiates the calculations. While the calculations are in progress a small window indicates the status. To stop the calculations, click the Cancel button. When the calculations are complete, a table displaying the results appears.



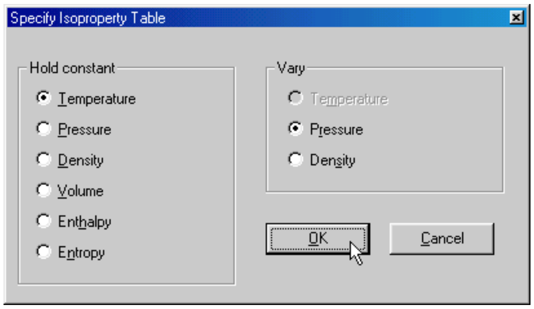
3: carbon dioxide: V/L sat. T=-100.00 to 100.00 °C

	Temperature (°C)	Pressure (MPa)	Liquid Density (kg/m³)	Vapor Density (kg/m³)	Liquid Enthalpy (kJ/kg)	Vapor Enthalpy (kJ/kg)	Liquid Cp (kJ/kg-K)	Vapor Cp (kJ/kg-K)	Liquid Therm. Cond. (mW/m-K)	Vapor Therm. C (mW/m-
1	-55.000	0.55397	1172.9	14.673	83.091	430.99	1.9569	0.91838	178.58	11.14
2	-50.000	0.68234	1154.6	17.925	92.943	432.68	1.9712	0.95194	172.06	11.57
3	-45.000	0.83184	1135.8	21.717	102.87	434.13	1.9892	0.98996	165.63	12.041
4	-40.000	1.0045	1116.4	26.121	112.90	435.32	2.0117	1.0333	159.30	12.54
5	-35.000	1.2024	1096.4	31.216	123.05	436.23	2.0393	1.0830	153.04	13.08
6	-30.000	1.4278	1075.7	37.098	133.34	436.82	2.0731	1.1406	146.86	13.68
7	-25.000	1.6827	1054.2	43.880	143.79	437.06	2.1145	1.2083	140.73	14.34
8	-20.000	1.9696	1031.7	51.700	154.45	436.89	2.1653	1.2893	134.64	15.09
9	-15.000	2.2908	1008.0	60.728	165.34	436.27	2.2283	1.3877	128.59	15.95
10	-10.000	2.6487	982.93	71.185	176.52	435.14	2.3072	1.5091	122.54	16.96
11	-5.0000	3.0459	956.21	83.359	188.05	433.38	2.4085	1.6628	116.50	18.171
12	0.00000	3.4851	927.43	97.647	200.00	430.89	2.5423	1.8648	110.43	19.671
13	5.0000	3.9695	896.03	114.62	212.50	427.48	2.7268	2.1440	104.31	21.601
14	10.000	4.5022	861.12	135.16	225.73	422.88	2.9976	2.5578	98.119	24.20
15	15.000	5.0871	821.21	160.73	239.99	416.64	3.4360	3.2371	91.862	27.961
16	20.000	5.7291	773.39	194.20	255.87	407.87	4.2637	4.5599	85.683	33.94

Sample saturation table.

5.2 Calculating Iso-Property tables

Selecting the Iso-Property Tables option in the Calculate menu starts calculation of a table with one property held constant and either the temperature, pressure, or density varied over a specified range. The following dialog allows the selection of the constant and varying properties. Click on one property from each list.



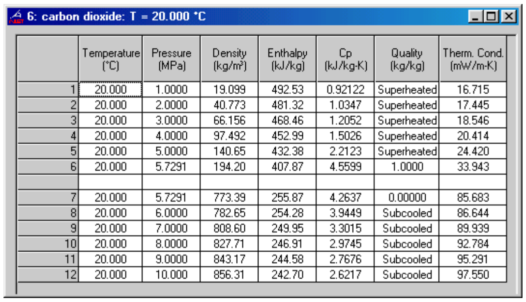
Specify Isoproperty Table

Hold constant
● Temperature
○ Pressure
○ Density
○ Volume
○ Enthalpy
○ Entropy

Vary
○ Temperature
● Pressure
○ Density

Clicking the OK button brings up a dialog for specifying the value of the property held constant and the range and increment of the varying property; this is the same dialog used with the saturation tables (see previous section). Default values are provided. The first time a table is calculated for a specific fluid, the defaults are based on the current units settings and the properties of the fluid or mixture. For subsequent calculations, the default range and increment are those from the previous table. The range and increment revert to the default values when a new fluid or mixture is specified. Deselecting the “Reset bounds...” option under Preferences retains the range and increment; see Section 7.5. The Leave active check box at the lower left keeps this dialog as the top window on the screen, allowing rapid calculation of a series of tables of the same type. Multiple tables generated from this procedure can be plotted together by selecting all the generated tables (hold down the shift key) in the New Plot menu (Section 6.1).

Clicking the OK button initiates the calculations. While the calculations are in progress a small window indicates the status; you can stop the calculations by clicking the Cancel button. When the calculations are complete, a table displaying the results appears. A blank line in the table indicates a change of phase.

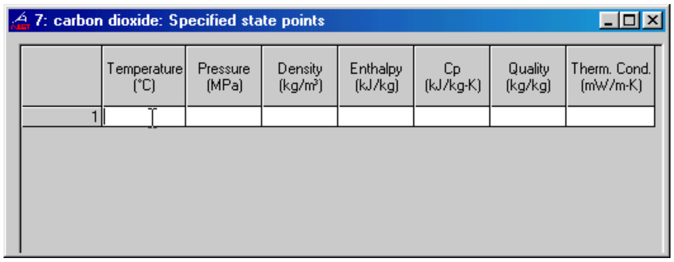


	Temperature (°C)	Pressure (MPa)	Density (kg/m³)	Enthalpy (kJ/kg)	Cp (kJ/kg-K)	Quality (kg/kg)	Therm. Cond. (mW/m-K)
1	20.000	1.0000	19.099	492.53	0.92122	Superheated	16.715
2	20.000	2.0000	40.773	481.32	1.0347	Superheated	17.445
3	20.000	3.0000	66.156	468.46	1.2052	Superheated	18.546
4	20.000	4.0000	97.492	452.99	1.5026	Superheated	20.414
5	20.000	5.0000	140.65	432.38	2.2123	Superheated	24.420
6	20.000	5.7291	194.20	407.87	4.5599	1.0000	33.943
7	20.000	5.7291	773.39	255.87	4.2637	0.00000	85.683
8	20.000	6.0000	782.65	254.28	3.9449	Subcooled	86.644
9	20.000	7.0000	808.60	249.95	3.3015	Subcooled	89.939
10	20.000	8.0000	827.71	246.91	2.9745	Subcooled	92.784
11	20.000	9.0000	843.17	244.58	2.7676	Subcooled	95.291
12	20.000	10.000	856.31	242.70	2.6217	Subcooled	97.550

Sample iso-property table calculated along an isotherm.

5.3 Calculating Tables at Specified State Points

The Specified State Points option calculates properties at arbitrary values of the independent variables (including composition). Selecting this option from the Calculate menu brings up a blank grid similar to a one-line spreadsheet.



	Temperature (°C)	Pressure (MPa)	Density (kg/m³)	Enthalpy (kJ/kg)	Cp (kJ/kg-K)	Quality (kg/kg)	Therm. Cond. (mW/m-K)
1							

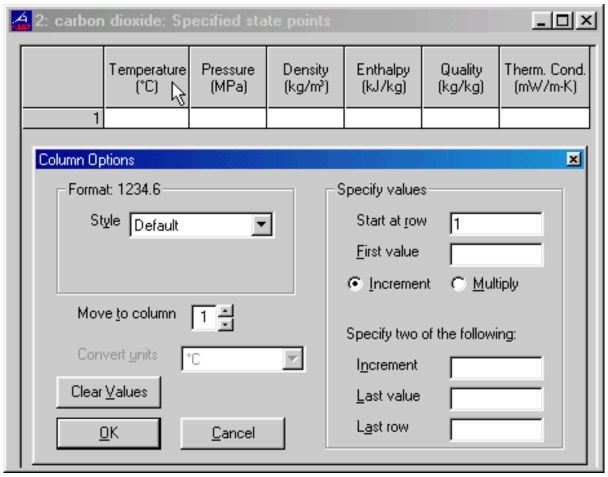
Empty specified state points table ready for input of independent variables.

The independent variables can be entered in a number of ways:

1. Values can be simply typed into the cells of the property table. You can move to any cell by clicking the mouse in that cell, or move among cells by pressing the Return, Tab, or arrow keys.

2. Values can be pasted into the independent variable cells from another application, such as a spreadsheet. Copy the values to the clipboard using the other application's Copy command. Then, in the property database, click the mouse in the first cell in the table and select the Paste command. Additional rows will be added automatically as needed.

3. Values can be automatically entered in a systematic manner by clicking on the header at the top of the column. This action brings up the Column options window



Format: 1234.6

Style: Default

Move to column: 1

Convert units: °C

Specify values

Start at row: 1

First value:

● Increment ○ Multiply

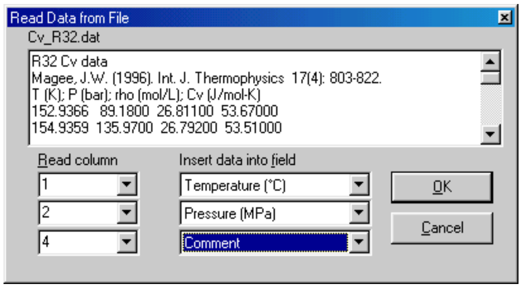
Increment:

Last value:

Last row:

Specify the starting value and starting row number in the boxes at the top right of the dialog. Then enter the specifications for the final row; note that only two of (increment, last value, last row) are needed. To enter a constant value, simply enter that value in the last row.

4. Values can be read from an ASCII file stored on disk. A specified state point table must be active before issuing this command. From the Edit menu select the Read Data From File command. A standard Open file dialog appears in which you may specify the file containing the independent property values. Select the file and the following dialog appears.



Cv_R32.dat

```
R32 Cv data
Magee, J.W. (1996). Int. J. Thermophysics  17(4): 803-822.
T (K); P (bar); rho (mol/L); Cv (J/mol-K)
152.9366   89.1800  26.81100  53.67000
154.9359  135.9700  26.79200  53.51000
```

Read column	Insert data into field
1	Temperature (°C)
2	Pressure (MPa)
4	Comment

The window displays the first 20 lines of the selected file in the box at the top of the window so that you can see the format of the values in the file. REFPROP will read one or more values from each line in the file and place them in corresponding lines in the blank Specified State Points table. Lines in the file which begin with any nonnumeric character are treated as comments and are ignored.

In the example shown here, temperature and pressure were chosen as the independent properties and are read from columns 1 and 2 of the file. It is not necessary to read all of the properties from the file; for example, you can read just the temperature by changing the second box to nothing.

The Read data from file option also allows you to read extra data from the file. This capability is useful, for example, in comparing experimental and calculated values of a property. In the example above, the experimental isochoric heat capacity is located in column 4. The comment field is selected in the third box. (See Preferences, Section 7.5, to add a comment column.) The data in this column of the file are read and placed in the comment column in the table. They can then be plotted, along with calculated values.

A combination of data entry methods can also be used. For example, Copy and Paste can be used to specify one of the independent variables while the other(s) are keyed in manually.

Whether the independent properties are read from a file or entered manually, as soon as any two valid input properties have been entered, the remaining properties will be calculated and displayed in the appropriate columns. The inputs can vary from row to row (for example, temperature and density for one row and temperature and enthalpy for the next), but not all combinations are supported. Note that you can then change the inputs or select new inputs (which causes the calculated values in that row to be erased) and repeat the calculation process.

For mixtures, the composition of the mixture can be entered on a line, but this must be done BEFORE the independent variables are entered. Otherwise the current mixture composition is used. For convenience, the “Specified State Points (varying composition)” command can be chosen. This command places the composition fields at the beginning of the table (and activates them if they were not selected among the properties to be displayed, see Section 7.3).

Saturation or melting line states can be calculated by adding the letters "l", "v", or "m" (designating a state point for the saturated liquid or vapor or along the melting line, respectively) after (or before) the value of temperature, pressure, density, enthalpy, or entropy. Note that "m" returns liquid properties at the solid-liquid boundary. REFPROP does not calculate solid properties. In the case where "l" or "v" is entered, and the entered value does not correspond to a valid liquid or vapor state point, the point is returned regardless of whether or not it is in the liquid or vapor state. For example, if a liquid density is entered with a "v", the liquid state is calculated internally, however, the equilibrium vapor state is displayed. The same is true for a vapor state entered with "l".

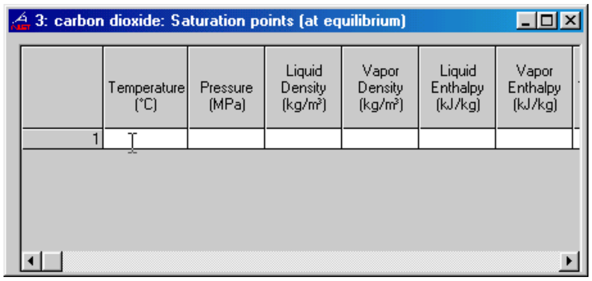
Saturation properties at specified points may also be calculated using the Saturation Points options as described below.

5.4 Calculating Saturation Properties at Specified Points

There are two options to calculate saturation properties at specified points in a manner similar to the Specified State Point options described in Section 5.3. They differ in the calculation basis used. For the “Saturation Points (at equilibrium)” option, the temperature and pressure of the two phases are the same, and the liquid and vapor compositions are in equilibrium, but the compositions are different (except for the special case of an azeotrope).

For the “Saturation Points (bubble and dew points at same composition)” option, the liquid and vapor are of the same composition, in which case the temperature or pressure of the liquid and vapor phases are not in equilibrium. This option is useful when working with a mixture of fixed composition. See also the discussion in Section 5.1.

Either of the Saturation Points options calculates properties at arbitrary values of an independent variable (plus optional composition). Selecting this option from the Calculate menu brings up a blank grid similar to a one-line spreadsheet.



3: carbon dioxide: Saturation points (at equilibrium)

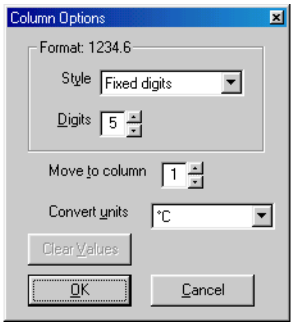
	Temperature (°C)	Pressure (MPa)	Liquid Density (kg/m³)	Vapor Density (kg/m³)	Liquid Enthalpy (kJ/kg)	Vapor Enthalpy (kJ/kg)
1						

Empty saturation points table ready for input of independent variables.

The independent variable(s) can be entered in the same ways as for the Specified State Points tables; see Section 5.3. The primary differences are that the Saturation Points tables will have a liquid and a vapor column for each property and only one independent variable is needed to specify the state. Enter a value for the liquid phase temperature, pressure, or density to specify conditions at the bubble point, or enter a value for the vapor phase temperature, pressure, or density to specify conditions at the dew point. For mixtures, the currently-defined composition is used for the calculations unless a different value is specified BEFORE the temperature, pressure, or density is entered. If composition is entered, take care that the phase specified for the composition and the independent variable are the same, otherwise the composition will revert to that for the currently defined mixture.

5.5 Reformatting Existing Data Tables

The property values are displayed in the calculated tables in a default format, which should be acceptable for most uses. The format of a column can be changed, or its position in the table shifted, by clicking on the column heading. This brings up the following dialog.



Format: 1234.6
Style: Fixed digits
Digits: 5
Move to column: 1
Convert units: °C

In addition to the default format, three other formats are accessible by clicking on the Style drop-down arrow. The “Fixed decimal” style displays values with a fixed number of digits after the decimal place. The “Fixed digits” style displays values with a fixed number of significant digits. The “Scientific notation” style displays values in scientific notation with a fixed number of digits in the ordinate. If either of these styles is selected, an edit box appears below the style. Select the desired number of digits by typing the value in the edit box, or using the small up or down arrows to increase or decrease the displayed value. An example of the selected format is shown above the style drop-down box.

The user is cautioned that, by the very nature of a calculational database, property data are often displayed with more digits than can be justified based on the accuracy of the property models or the uncertainties in the experimental data to which the models were fitted. A large number of digits may be useful for the smooth plotting of results, the evaluation of numerical derivatives, or checking results with the original source.

The position of a column in the table can be changed by editing the value in the edit box at the bottom of the dialog. The number of digits can be changed for all columns and all tables in the Preferences dialog under the Options menu, see Section 7.5.

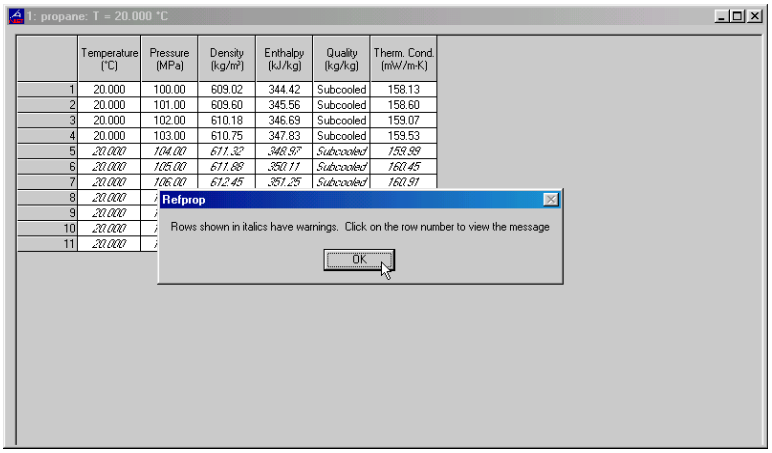
The width of the data columns can be changed by placing the mouse over the line separating the header of two columns. When the cursor changes to a double-headed arrow, click and drag the line to a new position. The column widths are also enlarged in some operations when the width of the numbers in the column exceeds the column width.

5.6 Warnings and Errors

It is not always possible to complete the requested property calculations. In such instances, the database returns a notation such as “not applicable” in a table cell, a warning message, or an error message.

Certain properties are not defined at states that are otherwise valid. For example, the viscosity and speed of sound are not defined for a two-phase state. The surface tension is not defined for single-phase states. In such cases the term “not defined” is displayed in the corresponding table cell(s), and the remaining properties are displayed normally. The quality can be defined in a variety of ways for subcooled liquid and superheated vapor states, and it is not defined for supercritical states. In these cases, the state (subcooled, superheated, or supercritical) is displayed in the table cell(s) for quality.

Warnings indicate a situation in which the calculated values may be suspect. The user is informed that one or more requested states has resulted in a warning by an Alert box, which is displayed after all calculations have been completed. The entire row in the table resulting in a warning is displayed in an italic font (even though the warning may arise from the calculation of a single property). You can view the warning message by clicking the affected row number(s).

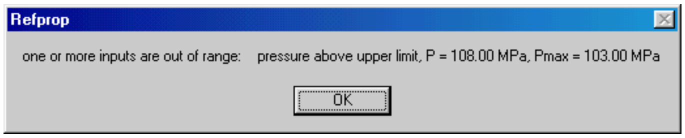


1: propane: T = 20.000 °C

	Temperature (°C)	Pressure (MPa)	Density (kg/m³)	Enthalpy (kJ/kg)	Quality (kg/kg)	Therm. Cond. (mW/m-K)
1	20.000	100.00	609.02	344.42	Subcooled	158.13
2	20.000	101.00	609.60	345.56	Subcooled	158.60
3	20.000	102.00	610.18	346.69	Subcooled	159.07
4	20.000	103.00	610.75	347.83	Subcooled	159.53
5	*20.000*	*104.00*	*611.32*	*348.97*	*Subcooled*	*159.99*
6	*20.000*	*105.00*	*611.88*	*350.11*	*Subcooled*	*160.45*
7	*20.000*	*106.00*	*612.45*	*351.25*	*Subcooled*	*160.91*
8	*20.000*					
9	*20.000*					
10	*20.000*					
11	*20.000*					

Refprop

Rows shown in italics have warnings. Click on the row number to view the message



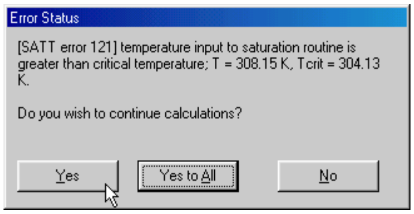
Refprop

one or more inputs are out of range: pressure above upper limit, P = 108.00 MPa, Pmax = 103.00 MPa

Warnings are most commonly encountered when transport property values are requested at a temperature and/or pressure outside of the range of the model used for the calculations. (The transport property models often have a more limited range than the corresponding thermodynamic property model; in these cases, the thermodynamic properties are calculated normally, but the transport properties generate a warning.) Warnings are also issued when the temperature and/or pressure are slightly above the stated limits of the equation of state.

An error indicates a situation in which calculations are not possible. This may be because of the failure of an iteration loop within the property routines to converge on a solution, but more commonly, is because states were requested for which calculations are impossible. For example, saturation calculations are not possible above the critical temperature. Also, while an equation of state can usually be extrapolated to slightly higher temperatures or pressures than the stated limits with good results, extrapolation to lower temperatures or higher densities can give nonsensical results and is not allowed.

When an error is generated by the property routines, an Alert box is immediately displayed giving the error message and the option to continue or cancel further calculations in the table. If the Yes button is clicked, calculations continue (although further errors are likely). The "Yes to All" button suppresses further error messages of the same type. If the No button is clicked, any rows calculated before the error was encountered are displayed, but no further calculations are attempted.



[SATT error 121] temperature input to saturation routine is greater than critical temperature; T = 308.15 K, Tcrit = 304.13 K.

Do you wish to continue calculations?

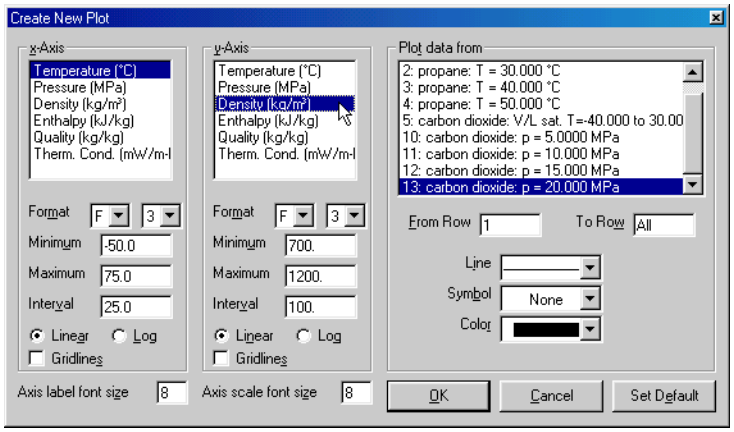
For further details on the warning and error messages generated by the database refer to Appendix E.

6. CREATING AND MODIFYING PLOTS
(The Plot Menu)

The REFPROP database provides a plotting capability for any data appearing in a table. In addition, simple plots of the thermodynamic surface can be easily generated on a wide range of coordinates, including temperature-entropy and pressure-enthalpy. Temperature-composition and pressure-composition diagrams for binary mixtures can be generated automatically. While these plotting capabilities help in the visualization of data trends and are adequate for many other purposes, the database is not intended to compete with programs devoted to plotting and data analysis. If you need to produce publication-quality plots or carry out statistical analyses or other data manipulations, we recommend that you transfer the property data from REFPROP to such a program. Section 9 of this manual describes the process to transfer data to other programs.

6.1 Plotting Data from Tables

Once one or more property tables have been calculated, x-y plots can be generated by the New Plot command. The dialog shown below is divided into three blocks, which control the x-axis, the y-axis, and the source and appearance of the plotted data.


Create New Plot

x-Axis
- Temperature (°C)
- Pressure (MPa)
- Density (kg/m³)
- Enthalpy (kJ/kg)
- Quality (kg/kg)
- Therm. Cond. (mW/m-

Format: F 3
Minimum: -50.0
Maximum: 75.0
Interval: 25.0
● Linear ○ Log
☐ Gridlines

y-Axis
- Temperature (°C)
- Pressure (MPa)
- Density (kg/m³)
- Enthalpy (kJ/kg)
- Quality (kg/kg)
- Therm. Cond. (mW/m-

Format: F 3
Minimum: 700.
Maximum: 1200.
Interval: 100.
● Linear ○ Log
☐ Gridlines

Plot data from
- 2: propane: T = 30.000 °C
- 3: propane: T = 40.000 °C
- 4: propane: T = 50.000 °C
- 5: carbon dioxide: V/L sat. T=-40.000 to 30.00
- 10: carbon dioxide: p = 5.0000 MPa
- 11: carbon dioxide: p = 10.000 MPa
- 12: carbon dioxide: p = 15.000 MPa
- 13: carbon dioxide: p = 20.000 MPa

From Row: 1
To Row: All
Line: ————
Symbol: None
Color: ■

Axis label font size: 8
Axis scale font size: 8

By default, it is assumed that data from the topmost table window are to be plotted. Other tables can be selected using the drop-down list at the upper right of the dialog. It is also assumed that all rows in the selected table are to be plotted. If this is not desired, the starting and ending row numbers can be entered in the edit boxes below the table list.

The variables to be plotted on the x- and y-axes are selected by clicking the column headings listed in the scroll boxes at the left and middle of the dialog.

Data from multiple tables can be plotted simultaneously by selecting multiple items in the 'Plot data from' list and pressing 'OK'. You must be careful that the selected items all contain the same columns. Plotting data from isoproperty tables and saturation tables together must be done in two steps (once with New Plot, then with Overlay Plot).

Minimum and maximum values for the plot frame are generated as the x- and y-variables are selected. The Interval value represents the spacing of axis tic marks. These values can be changed by typing new values; they can also be changed later using the Modify Plot command, which is described below. The format of the axis labels is controlled by two small drop-down boxes. The first provides access to a fixed decimal format, “F”, or exponential notation, “E”. The second Format drop-down box controls the number of digits to be displayed after the decimal point with either format. Either a linear or logarithmic axis scaling can be specified by the radio buttons at the bottom of the dialog. Finally, a check box turns grid lines on or off.

The appearance of the plotted points is controlled by the commands in the lower right portion of the dialog. Points can be connected by a variety of line types, or no line at all, by selecting the desired option in the drop-down list labeled “Line.” The “Symbol” drop-down list gives you access to a variety of plotting symbols, including no symbol. (The choice of “none” for both the line type and symbol is allowed, but this results in a rather uninteresting plot.) The color of both the line and symbol is also controlled by a drop-down list. The default values for these attributes can be saved by clicking the Save Defaults button.

6.2 Overlaying Data Onto Existing Plots

You can plot additional data onto existing plots by using the Overlay Plot command. The command acts on the topmost plot window; if a different plot is desired, select it before executing the Overlay Plot command. This command brings up a dialog virtually identical to that for New Plot, and it works in the same way. Overlaid plots use the existing scales for the ordinate and abscissa. However, if the overlaid plot has values that cause part or all of the plot to be off scale, a dialog is presented which asks if you want to rescale the plot. It is the user's responsibility to ensure that plots are not overlaid in meaningless combinations. In particular, the quantities in the individual data sets plotted should have the same units.

6.3 Predefined Diagrams

A number of common diagrams are predefined in the database and can be automatically generated for the currently defined fluid or mixture. Once plotted, these predefined plots can be modified, or additional data can be overlaid on them, in the same fashion as for any other plot.

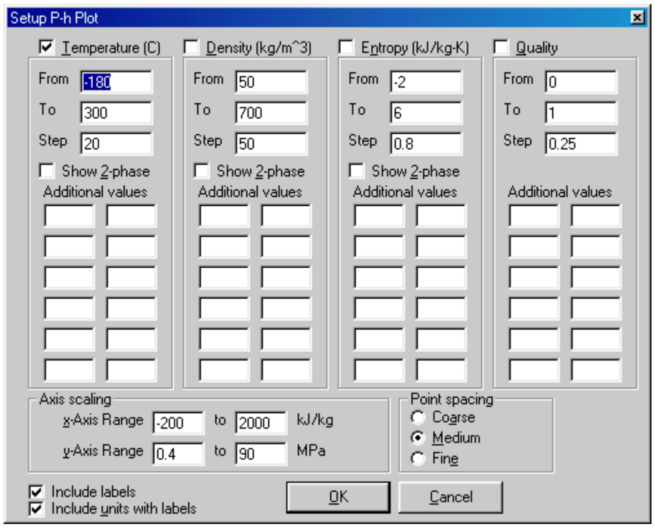
6.3.1 Diagrams of thermodynamic surfaces

Skeleton diagrams of the thermodynamic surface of the current fluid or mixture can be generated. The types of diagrams that can be plotted include:

Temperature vs. Entropy
Temperature vs. Enthalpy
Pressure vs. Enthalpy
Pressure vs. Density
Pressure vs. Volume
Compressibility Factor vs. Pressure
Enthalpy vs. Entropy
Isochoric Heat Capacity vs. Temperature
Isobaric Heat Capacity vs. Temperature
Speed of Sound vs. Temperature
Energy vs. Enthalpy

Also, plots of the transport properties of viscosity and thermal conductivity can be generated in a similar fashion.

Selecting any of these options brings up a dialog in which the properties to be plotted can be specified as shown below.



Setup P-h Plot

☑ Temperature (C): From -180, To 300, Step 20, ☐ Show 2-phase

☐ Density (kg/m^3): From 50, To 700, Step 50, ☐ Show 2-phase

☐ Entropy (kJ/kg-K): From -2, To 6, Step 0.8, ☐ Show 2-phase

☐ Quality: From 0, To 1, Step 0.25

Axis scaling
x-Axis Range -200 to 2000 kJ/kg
y-Axis Range 0.4 to 90 MPa

Point spacing
○ Coarse
● Medium
○ Fine

☑ Include labels
☑ Include units with labels

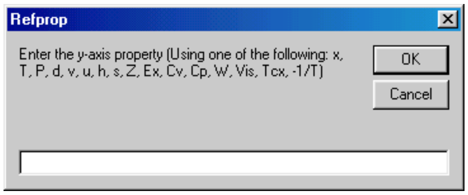
Each diagram type will allow different combinations. In the example shown, a pressure vs. enthalpy diagram can display lines of constant temperature, density, entropy, and/or quality. The saturated liquid and saturated vapor lines are always calculated. To plot a property, place a check in the box to the left of the label. You can then specify a range of values to be plotted or up to 10 individual values, or both.

The minimum and maximum values of the x and y axis can be modified. These values can also be changed later with the Modify Plot command, however, some data may not be calculated beyond the ranges indicated in these boxes, and a new diagram will have to be generated with larger bounds.

Labels identifying the isoproperties are automatically generated if the “Include labels” option is selected. The number of data points calculated, resulting in smooth or segmented lines, can be selected in the “Point spacing” option.

In addition, values in the two-phase region can also be plotted by use of the “Show 2-phase” check box. By default, this option is not selected, and a straight line is drawn between the saturated liquid state and the saturated vapor state. For mixtures, showing two-phase values will be very computationally intensive. When plotting isotherms for a pure fluid, the two-phase option works differently than might be expected: values of the metastable states are shown, both real, and inaccessible. However, you should realize that there are virtually no metastable data for most fluids, and values shown will be extrapolations of the equations of state. Indeed, a major use of this option is to examine the behavior of equations of state. In addition, calculated values can be extremely large, and plotting these values can result in unexpected plots of the two phase.

A large number of other diagrams can be generated in a similar fashion by the “Other diagrams” option in the Plot menu. This option brings up the following dialog:

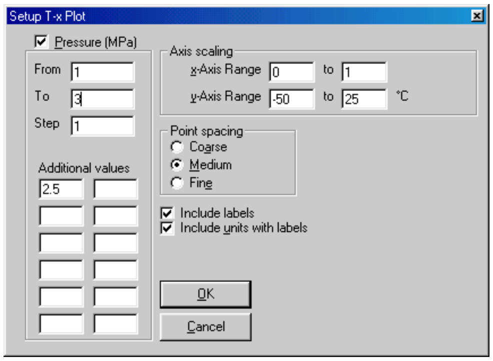


Enter the y-axis property (Using one of the following: x, T, P, d, v, u, h, s, Z, Ex, Cv, Cp, W, Vis, Tcx, -1/T)

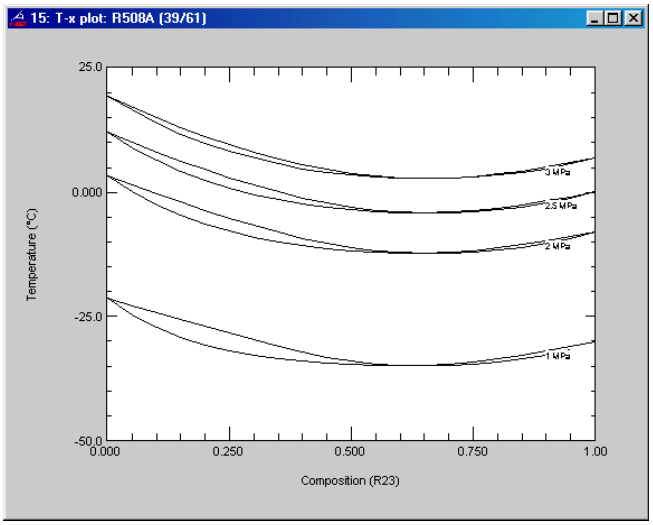
Enter the desired property for the y-axis using the abbreviations listed; then click the OK button (or hit Enter). A similar dialog appears to specify the x-axis property. Once both coordinates are selected, a dialog identical to that for the predefined surfaces appears.

6.3.2 Phase diagrams

A phase diagram plotting bubble (saturated liquid) and dew (saturated vapor) lines as functions of temperature and composition for constant values of pressure is generated by the T-x Diagram command. The P-x Diagram command generates a similar diagram on pressure-composition coordinates for constant values of temperature. These options are available only for binary mixtures; the commands are dimmed for pure fluids and for mixtures with three or more components. The dialog shown below allows specification of a range of pressures (or temperatures for the P-x diagram) to be plotted.



☑ Pressure (MPa)
From 1
To 3
Step 1
Additional values 2.5
x-Axis Range 0 to 1
y-Axis Range -50 to 25 °C
○ Coarse
● Medium
○ Fine
☑ Include labels
☑ Include units with labels

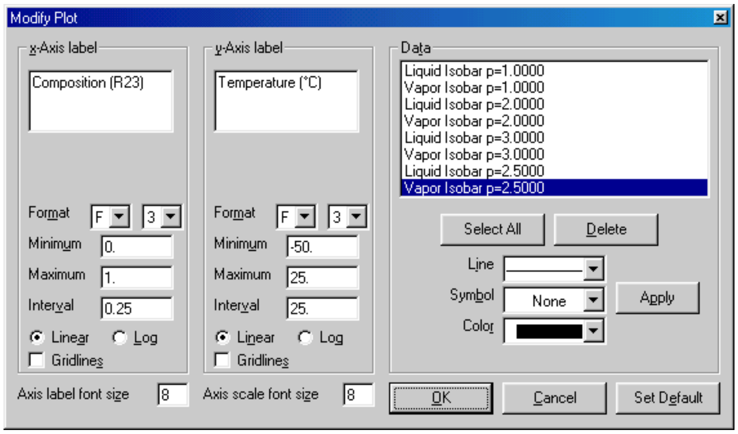


6.4 Modifying Plots

6.4.1 The Modify Plot command

Many of the attributes of a plot can be changed through the Modify Plot command. This command can be accessed by the pull-down menu item or by double-clicking anywhere within an existing plot. In the former case, the plot in the topmost window is affected. If the topmost window is not a plot the most recent plot is acted on.

The dialog for this command is similar to that used to specify a new plot, except that the variables plotted cannot be changed (although the x- and y-axis labels can be edited). As with the New Plot command, linear or logarithmic scaling can be selected, and the plot limits and axis label formats can be changed. Options to modify the size of the axis labels and add gridlines to the plot are provided in the “X-Axis” and “Y-Axis” portions of the dialog.



x-Axis label: Composition (R23)
Format: F 3
Minimum: 0.
Maximum: 1.
Interval: 0.25
● Linear ○ Log
☐ Gridlines
Axis label font size: 8

y-Axis label: Temperature (°C)
Format: F 3
Minimum: -50.
Maximum: 25.
Interval: 25.
● Linear ○ Log
☐ Gridlines
Axis scale font size: 8

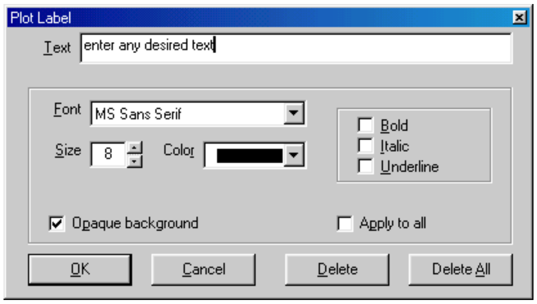
Data:
Liquid Isobar p=1.0000
Vapor Isobar p=1.0000
Liquid Isobar p=2.0000
Vapor Isobar p=2.0000
Liquid Isobar p=3.0000
Vapor Isobar p=3.0000
Liquid Isobar p=2.5000
Vapor Isobar p=2.5000

Line: ———
Symbol: None
Color: ■

A drop-down box in the upper right lists the individual data sets plotted. Selecting an item allows editing of the line and symbol attributes for that data set. The Delete button permanently deletes the selected data set. (Note that for the predefined plots, there is an entry for each of the lines comprising these diagrams.) Select the data set for which the line type, symbol, and/or color specifications are to be applied. These changes can be made to one data set at a time or to a multiple selection (by shift-clicking). After changes have been made, either the Apply button or the OK button can be selected. By pressing the Apply button, other changes can be made as well. The Delete button removes all selected datasets from the plot.

6.4.2 Adding and deleting labels

The Add Label command places text in a plot window. A plot must be in the foremost window for this command to be active. Invoking this command brings up a dialog in which you can type the desired text. Other text characteristics including the font, size, and color can also be edited. The “Opaque background” option is invoked by a check box; when this option is turned on, any lines “underneath” a text label are blocked out.



Plot Label

Text: enter any desired text

Font: MS Sans Serif

Size: 8

☐ Bold
☐ Italic
☐ Underline

☑ Opaque background

☐ Apply to all

You can modify an existing label (including those generated through the predefined plots) by double-clicking within the boundaries of the text. A label can be permanently deleted with the Delete button. The Delete All button deletes all of the labels on a plot.

Labels can be moved by clicking within the text boundaries and dragging the text to its new location.

6.4.3 Resizing and moving plots

The size of the plot frame can be changed. Place the cursor over the lower right corner of the plot window; the cursor changes to a double-ended arrow to indicate that you are in the resize mode. Click and hold the mouse button while dragging the corner of the plot to enlarge or reduce the plot size.

6.4.4 Reading coordinates off a plot

You can display the (x, y) coordinates of any point within the plot frame. Press the Shift key to display cross hairs within the plot frame and numerical coordinates (in units corresponding to the plot axes) appear in the title bar of the plot window. Use the mouse to move the cross hairs to any desired point in the plot.

6.4.5 Zooming

The area displayed in a plot can be changed. Click and drag the left mouse button to create a box. When the mouse button is released, the area within the box will become the new plotted area. The plot area can also be zoomed in or out by a factor of two with the Zoom In and Zoom Out options in the Plot menu. The Zoom Full Frame option returns the plot to its original bounds set by New Plot or Modify Plot.

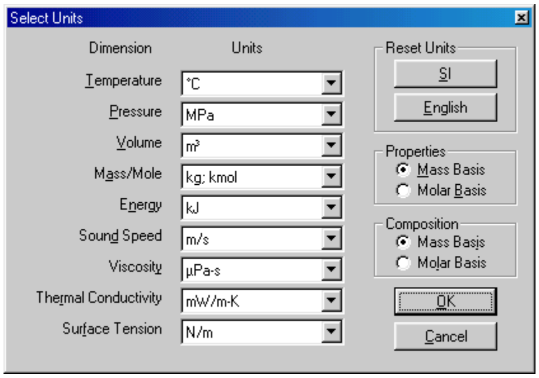
7. CHANGING OPTIONS AND PREFERENCES

(The Options Menu)

Under the Options menu, you can choose the units of measure for the calculations, the reference state for enthalpy and entropy, the properties to be displayed, and other options. All of these options can be saved (together with the currently defined fluid or mixture) for use in a future session. Any changes in these options apply to all subsequent tables but do not affect any existing tables (with one exception, as explained below).

7.1 Units

The Units command brings up a dialog in which the units of the various properties can be specified. The current settings are displayed down the left side of the dialog window. Some properties use combinations of the displayed settings and cannot be specified independently. For example, if kilograms and kilojoules are specified for mass and energy, respectively, enthalpy is displayed in units of kJ/kg.



Dimension	Units
Temperature	°C
Pressure	MPa
Volume	m³
Mass/Mole	kg; kmol
Energy	kJ
Sound Speed	m/s
Viscosity	µPa-s
Thermal Conductivity	mW/m-K
Surface Tension	N/m

Properties
● Mass Basis
○ Molar Basis

Composition
● Mass Basis
○ Molar Basis

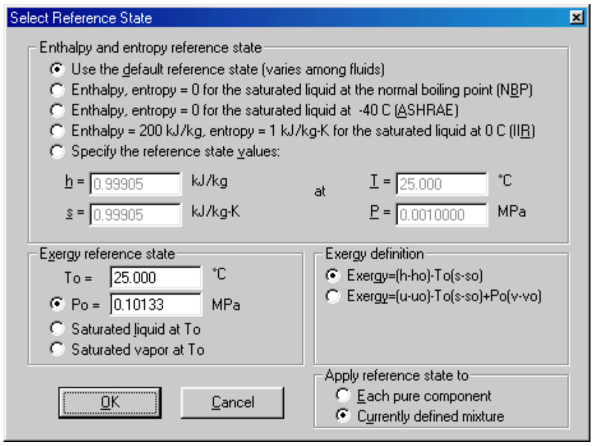
Click the SI or English buttons to set/reset all of the units to one of these unit systems. Units can also be set individually—click on the arrow to the right of the current unit setting. A drop-down list of available choices appears. Click the desired unit.

Specific properties (*i.e.,* those expressed in terms of a unit quantity) are reported on either a mass or molar basis (*e.g.,* kJ/kg or J/mol). Select the desired basis by the radio buttons under the heading “Properties.” The size (prefix) of the molar and mass bases are governed by the selection in the Mass list box and are selected together. For example, selecting “kg; kmol” specifies kilograms if the mass basis is selected and a kilomole (often called a kilogram mole) for the molar basis; selecting the English units “lb; lb mol” specifies pounds and pound moles.

The basis for the compositions is specified independently of the mass or molar basis for the specific properties by the radio buttons at the lower right of the dialog. This allows you to, for example, specify a mixture composition on a mole fraction basis and display the properties on a mass basis.

7.2 Enthalpy and Entropy Reference States and Exergy

The properties of enthalpy and entropy are computed as differences relative to some arbitrary reference state. The Reference State command allows the selection of one of three conventions:



Enthalpy and entropy reference state
- ● Use the default reference state (varies among fluids)
- ○ Enthalpy, entropy = 0 for the saturated liquid at the normal boiling point (NBP)
- ○ Enthalpy, entropy = 0 for the saturated liquid at -40 C (ASHRAE)
- ○ Enthalpy = 200 kJ/kg, entropy = 1 kJ/kg-K for the saturated liquid at 0 C (IIR)
- ○ Specify the reference state values:

h = 0.99905 kJ/kg at T = 25.000 °C
s = 0.99905 kJ/kg-K P = 0.0010000 MPa

Exergy reference state
To = 25.000 °C
- ● Po = 0.10133 MPa
- ○ Saturated liquid at To
- ○ Saturated vapor at To

Exergy definition
- ● Exergy=(h-ho)-To(s-so)
- ○ Exergy=(u-uo)-To(s-so)+Po(v-vo)

Apply reference state to
- ○ Each pure component
- ● Currently defined mixture

1. The “normal boiling point” (NBP) choice sets the enthalpy and entropy to zero for saturated liquid at the normal boiling point temperature.

2. The choice of zero for enthalpy and entropy for the saturated liquid at –40 °C (= –40 °F) corresponds to the reference state traditionally used for refrigerants in the United States, including the tabulations of the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE).

3. The International Institute of Refrigeration (IIR) has adopted reference state values of 200 kJ/kg and 1 kJ/(kg-K) for enthalpy and entropy, respectively, for the saturated liquid at 0°C. ASHRAE also uses this reference state for most refrigerants in its tables in SI units.

A user-specified reference state can also be selected. If that radio button is selected, the four edit boxes underneath it become active. Enter the desired values of enthalpy (h) and entropy (s) at the reference state temperature (T) and pressure (P) into the edit boxes.

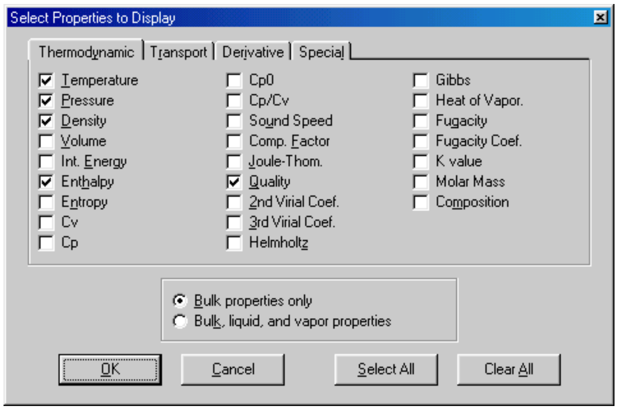
All of the above reference states may not be applicable to a given fluid. For example, the IIR and ASHRAE reference states specify a reference temperature above the critical temperature for methane. A reference state that does work is stored in the data file for each fluid. This reference state will be read from the file and applied if the choice “Use the default reference state” is selected.

For mixtures, any of the above reference states can be applied to each of the pure components individually or to the currently defined mixture by selecting the appropriate radio button at the bottom right of the dialog. If the pure component option is selected, the enthalpy and entropy of a mixture differs from the selected convention by amounts equal to the enthalpy and entropy of mixing. The mixture option is convenient when working with a refrigerant blend of specified composition. With this option the reference conventions are applied to liquid at the bubble point.

The reference state dialog also specifies the conventions used for exergy. Exergy is a specialized property which is used in reversibility analyses of thermodynamic cycles. Exergy values are referenced to a “zero” state, which is often taken to be ambient conditions. The reference or zero state temperature is specified by entering a value in the “To =” edit box. This zero-point temperature may be then associated with a zero-point pressure or the saturation state of the fluid by selecting among the radio buttons. Two definitions of exergy are in common use; the desired definition is selected by the radio buttons at the lower right of the dialog.

7.3 Properties Calculated

The properties to be displayed in calculated tables are controlled by the Properties dialog. The properties are organized into categories which are accessed by the tabs at the top of the dialog. Click on the desired category tab and select or deselect any property by clicking the check box next to its name. All of the properties for the displayed category may be selected or deselected by the “Select All” or “Clear All” buttons at the lower right.



☑ Temperature
☑ Pressure
☑ Density
☐ Volume
☐ Int. Energy
☑ Enthalpy
☐ Entropy
☐ Cv
☐ Cp
☐ Cp0
☐ Cp/Cv
☐ Sound Speed
☐ Comp. Factor
☐ Joule-Thom.
☑ Quality
☐ 2nd Virial Coef.
☐ 3rd Virial Coef.
☐ Helmholtz
☐ Gibbs
☐ Heat of Vapor.
☐ Fugacity
☐ Fugacity Coef.
☐ K value
☐ Molar Mass
☐ Composition

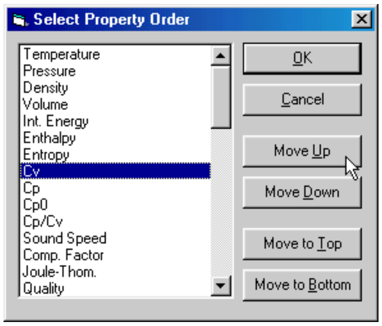
● Bulk properties only
○ Bulk, liquid, and vapor properties

In the lower part of the dialog, a pair of radio buttons controls whether properties for the liquid and vapor phases are to be displayed in addition to bulk properties. Liquid-phase properties are denoted by “Liquid” or “Liquid phase” in the table heading; “Vapor” or “Vapor phase” denotes the vapor-phase properties. The bulk properties have neither designation. For single-phase states, the bulk properties are the same as either the liquid- or vapor-phase properties, and either the liquid or vapor states are listed as “not applicable.” For two-phase states, the properties of the overall or bulk state are a combination of the saturated liquid and saturated vapor properties. Note that some properties, including speed of sound and viscosity, are not defined for two-phase states. (For saturation tables, this choice affects only tables with quality as the independent variable. For other types of saturation tables, the saturated liquid and saturated vapor properties are always displayed.)

The thermodynamic properties include pressure, density, heat capacity, etc. The transport properties include viscosity and thermal conductivity; surface tension is located here although it is not strictly a transport property. The “Derivative” properties include numerous partial derivatives of properties with respect to temperature, pressure, or density. The “Special” category includes exergy and the inverse temperature. Also included in the Special category are a number of properties listed as functions of (T, rho). These properties are calculated strictly as a function of the temperature and bulk density in any two-phase state; thus they represent metastable and unstable states. In single-phase states, these properties are the same as the corresponding “normal” properties.

7.4 Property Order

The property order dialog, shown below, establishes the order the properties are displayed in a table.



Select the property that you wish to move, and use the “Move up”, “Move down”, “Move to top,” or “Move to bottom” buttons to change the position of that property in any subsequent tables.

The property order can also be changed by selecting a property with the up and down arrow keys or the mouse, and then moving the property using the up and down arrow keys while holding down the shift key.

7.5 Preferences

The Preferences item in the Options menu brings up a dialog in which you can specify the behavior of the database in a number of aspects. Clicking on the check box next to the item activates or deactivates that option.

☐ Prompt to save session when closing
☑ Prompt before deleting row
☐ Ignore all error messages
☐ Ignore all warning messages
☑ Copy table headers to clipboard with table data
☑ Show saturation boundaries in tables
☐ Add a comment column to tables
☐ Use steam conversion value for Btu and cal
☐ Use nonstandard symbols (degree sign, etc.)
☑ Reset bounds when units or fluid are changed
☐ Flip usage of commas and periods in numbers
☐ Automatically hide banner screen on startup

5 Number of digits
Fixed digits Style
☐ Apply to existing tables

7 Table font size
☐ Apply to existing tables

If the “Prompt to save session when closing” option is selected, you will be prompted when the program is terminated to save the session to a file before closing. This file can then be retrieved using the Open Session command (Section 8.2) when the program is run again.

The “Prompt before deleting row” option prompts you before a row is deleted in a table (by either pressing Shift-del or selecting the Delete Row option while editing a table). A row cannot be recovered after it has been deleted.

The “Ignore all error messages” option will cause all error messages to be ignored that occur during property calculations. While this option may relieve you of having to clear such error messages, it may cause confusion when properties are not returned after entering inputs out of range or when the program does not converge.

The “Copy table headers to clipboard with table data” option can be used to select whether or not the headers at the top of each table are included when copying data to the clipboard (Section 9.1). (Table headers from REFPROP tables are automatically suppressed when you paste data into a Selected State Points table.)

When the “Show saturation boundaries in tables” option is selected, a blank line will appear between the single and two-phase state points and the boundary between the liquid and vapor phases in subsequent tables.

The option to add a comment column to tables will add an extra column in each table. The extra column can be used to enter comments or user data. The values in this field will be ignored in calculations, but numerical values can be plotted in the same manner as calculated properties. Adding text in each field can aid you in labeling each state point, and the size of the comment field can be enlarged by clicking and dragging the mouse as described in Section 5.5. A comment column is put at the end of the table by default, but this can be changed under Property Order as described in Section 7.4.

The steam conversion option will use the conversion 1 cal = 4.184 J when not selected, and the conversion 1 cal = 4.1868 J when selected. The later value is generally used only with the calculation of water and steam properties. The former value (4.184) should be used with all other fluids and mixtures.

In certain applications, such as using Japanese settings with Microsoft Windows, the degree sign, the superscript 2, and the superscript 3 will not be properly displayed, causing unit conversions to not work and displaying units with odd symbols. In such cases, the nonstandard characters should be turned off, resulting in the loss of the degree signs. The text '^2' and '^3' will be used in place of the superscript 2 and 3.

The default bounds used for the independent variables in calculating tables normally changes when the fluid or unit system is changed. By deselecting the “Reset bounds...” option, the previous bounds are retained. This is useful if you are wanting to compare properties for several fluids over similar ranges of conditions.

The “Flip usage of commas and periods in numbers” option allows REFPROP to conform to either the European or American convention for the decimal point. REFPROP will, however, usually recognize a users system settings, and this option will not be required.

In addition to these options, the number of digits in the tables and the font size used for the tables can be selected on a global basis, rather than by individually selecting the number of digits as described in Reformating Existing Data Tables (Section 5.5). Changes in the number of digits displayed will be applied to currently displayed tables if the “Apply to existing tables” option is selected. The “Fixed decimal” style displays values with a fixed number of digits after the decimal place. The “Fixed digits” style displays values with a fixed number of significant digits. The “Scientific notation” style displays values in scientific notation with a fixed number of digits in the ordinate. If either of these styles is selected, an edit box appears below the style. Select the desired number of digits by typing the value in the edit box, or using the small up or down arrows to increase or decrease the displayed value.

The preferences are saved when the Save Current Options command is issued (see next section). They are restored to a previously saved option with the Retrieve Options command see Section 7.7).

7.6 Saving Current Options and Preferences

The current settings can be saved at any time for recall. The settings saved include the currently defined fluid or mixture, units of measure, the reference state for enthalpy and entropy, the properties to be displayed, and the options specified in the Preferences dialog. Selecting the Save Current Options command brings up a file save dialog in which you can specify the filename to contain the current settings. Settings files are identified with the ".prf" file name extension. You can save multiple settings files corresponding to different projects, etc.

The database reads the settings file "defaults.prf" at startup. If you want to have the current options used as the default settings, save them in the "defaults.prf" file. An Alert box informs you that the file already exists and asks if you want to replace the existing file; click Yes to save the new defaults. To start REFPROP with a different preferences file, include the name of that file on the command line used to start REFPROP.

WARNING: Do not delete the "defaults.prf" file. This file is needed to start the program, and if it is missing, the program will revert to internal defaults (which will probably not correspond to your preferences), except that no fluid will be defined. If you inadventently delete the "defaults.prf" file you can rename another settings file to "defaults.prf" and place it in the same directory as the REFPROP executable. You will need to check and, if necessary, change all the settings.

7.7 Retrieving Previously Defined Options

Any previously stored settings can be loaded by executing the Retrieve Options command. This brings up a File Open dialog. The settings files are identified by a ".prf" filename extension. Select the name of the desired settings file and click OK to load those previously defined settings including the fluid or mixture, units of measure, the reference state for enthalpy and entropy, the properties to be displayed, and the options specified in the Preferences dialog.

8. SAVING AND PRINTING
(The File Menu)

8.1 Saving and Closing Sessions

A session in the REFPROP database consists of all table and plot window(s) on the screen together with the settings defining the fluid, unit system, reference state, and selected properties used to generate those windows. You can save a session at any time. This means that the complete current state of the program is saved to disk. The Save Session command brings up a File dialog. Select the desired directory and enter a filename; the ".rfp" file-type extension identifies a file as a REFPROP session file to the database.

The Close Session command closes all table and plot windows currently on the screen, but the database itself remains running. If you have not already saved the session, a dialog asks if you want to save the current session before closing (unless you have disabled this reminder under the "Preferences" dialog).

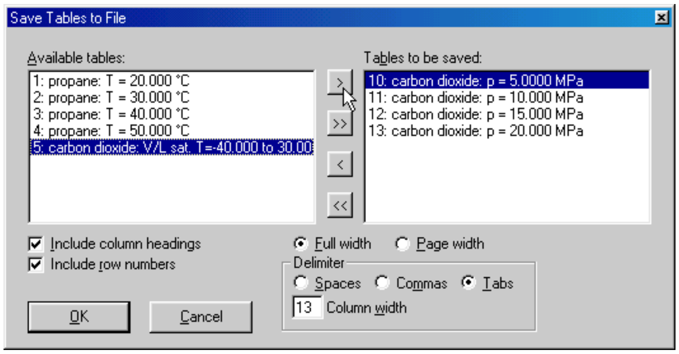
8.2 Retrieving a Previously Saved Session

A previously saved session can be retrieved by the Open Session command. This command, combined with Save Session, is a very powerful combination that allows you to stop work on a REFPROP analysis and return to it later or work simultaneously on several different analyses at one time.

The Open Session command brings up a File dialog where you specify the file storing the desired session. Upon pressing the OK button, the specified session is restored with all of its constituent table and plot window(s) on the screen. The settings defining the fluid, unit system, reference state, and selected properties used to generate those windows are also restored. Opening a saved session will delete any current windows; in this case an alert box will ask if you wish to proceed.

8.3 Saving Tables

The Save Tables command displays a dialog that allows you to select one or more of the current tables to be saved to disk in an ASCII format. The available tables are shown in the list at the left, with the most current one shown on the right. Click on the name of the table you want to save and then click on the ">" button to add that table to the list of tables to be saved on the right. The ">>" button moves all of the available tables to the right list. You can remove a table from the "to be saved" list by highlighting its name and pressing the "<" button. Similarly, all of the tables can be removed by pressing the "<<" button.



Available tables:

1: propane: T = 20.000 °C
2: propane: T = 30.000 °C
3: propane: T = 40.000 °C
4: propane: T = 50.000 °C
5: carbon dioxide: V/L sat. T=-40.000 to 30.00

Tables to be saved:

10: carbon dioxide: p = 5.0000 MPa
11: carbon dioxide: p = 10.000 MPa
12: carbon dioxide: p = 15.000 MPa
13: carbon dioxide: p = 20.000 MPa

☑ Include column headings
☑ Include row numbers

● Full width ○ Page width

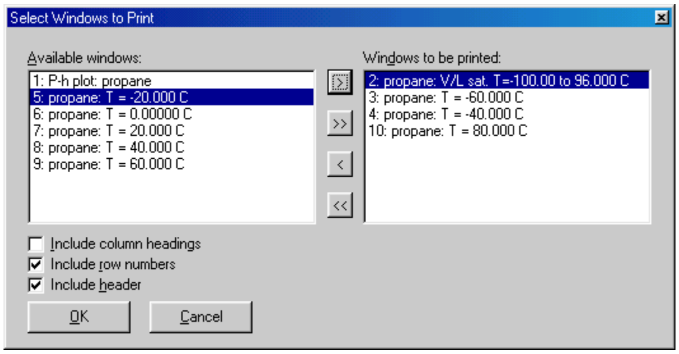
Delimiter
○ Spaces ○ Commas ● Tabs
13 Column width

The check boxes at the lower left gives you the option to include the column heading (consisting of the property and units on separate lines) and/or the row numbers together with the data. A delimiter selected by the radio buttons at the lower right is placed between each value in a row. Most spreadsheet programs use the tab character to place items in separate cells, for example. A carriage return is placed at the end of the row. When saving tables, the “Full width” option prints one line of the table on one line of the file; this can result in very long lines. The “Page width” option formats the tables so that all the properties fit within 80 columns in the file. The lines are broken up and printed in different sections, similar to that done during printing. Multiple tables, if specified, are saved to a single file. The tables in the selected list are saved or printed in the order in which they appear in the list.

8.4 Printing

The Print Setup command brings up the standard Print Setup dialog that gives you access to print options, such as landscape or portrait format and printer selection. These options are applied to subsequent output from the Print command. This command need only be used when the default printer or printer options are to be viewed or changed.

The Print command allows any of the tables or plots to be printed. The available windows are shown in the list at the left, with the most current one shown on the right. Click the name of the table or plot you want to print and then click the “>” button to add that window to the list on the right. The “>>” button moves all of the available windows to the right list. You can remove an item from the “print” list by highlighting its name and pressing the “<” button. Similarly all of the tables and plots can be removed by pressing the “<<” button. Clicking OK initiates the print process.



Available windows:

1: P-h plot: propane
5: propane: T = -20.000 C
6: propane: T = 0.00000 C
7: propane: T = 20.000 C
8: propane: T = 40.000 C
9: propane: T = 60.000 C

Windows to be printed:

2: propane: V/L sat. T=-100.00 to 96.000 C
3: propane: T = -60.000 C
4: propane: T = -40.000 C
10: propane: T = 80.000 C

☐ Include column headings
☑ Include row numbers
☑ Include header

The check boxes at the lower left allow you to include the column headings (containing the property names and units) and/or the row numbers on the printed output of tables. The “Include header” check box will also print out the window header containing the date, time, etc. Multiple tables or plots are printed in the order they appear in the “to be printed” list.

8.5 Exiting REFPROP

The Exit command provides a graceful way to exit from the program (quit). You are prompted to apply Save Session if it has not already been saved (unless this prompt has been turned off under the Preferences command, see Section 7.5). Memory allocated by the program is released.

9. IMPORTING AND EXPORTING DATA
(The Edit Menu)

9.1 Copying Data or a Plot to the Clipboard

The Copy Table Data and Copy Plot commands can be used to copy a plot or selected data from an existing window to the Clipboard. (The Clipboard is an area of memory used to exchange data within and between applications.) It can then be pasted into another application, such as a word processor or spreadsheet.

To copy a plot, bring the desired window to the front by clicking on it or by selecting its name under the Windows menu. Then select the Copy Plot command. The plot is placed on the Clipboard as a bitmap graphic, which can be pasted into most applications.

To copy data, it is first necessary to select the cells to be copied. To select a block of data, click the cell at one corner of the block, then press Shift and click at the diagonally opposite corner of the block. You can also select a block by clicking and dragging the mouse over it. You can also select the entire table by choosing Select All command under the Edit menu.

Once a block of data is selected, executing the Copy Table Data command copies it to the Clipboard. The table headings may also be copied along with the data, depending on the setting in the Preferences dialog (see Section 7.5).

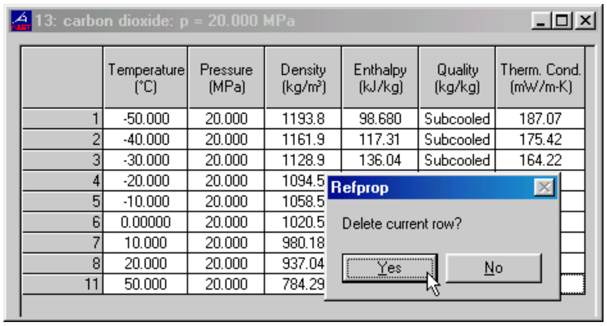
The Save Tables command provides another way to exchange data with other applications; see Section 8.3.

9.2 Pasting Data from the Clipboard

The Paste command places the contents of the Clipboard into the currently active input cell or edit box. This capability can be used to copy individual items, but is most useful in filling in the independent variables in a "Specified State Points" or "Saturated Points" table. To paste data into such a table, first click the top-left cell of the block into which you wish to place the Clipboard data, then choose Paste from the Edit menu. Entries in the same row must be separated by the tab character and a carriage return character must be used to delineate rows. (This is the format used by the REFPROP Copy command, and it is the norm for data copied to the Clipboard by most spreadsheet applications.)

9.3 Deleting a Row of Data

The Delete Row command (or the shift-del key stroke) allows a specified row (including its row number) to be permanently removed from a data table.



13: carbon dioxide: p = 20.000 MPa

	Temperature (°C)	Pressure (MPa)	Density (kg/m³)	Enthalpy (kJ/kg)	Quality (kg/kg)	Therm. Cond. (mW/m-K)
1	-50.000	20.000	1193.8	98.680	Subcooled	187.07
2	-40.000	20.000	1161.9	117.31	Subcooled	175.42
3	-30.000	20.000	1128.9	136.04	Subcooled	164.22
4	-20.000	20.000	1094.5			
5	-10.000	20.000	1058.5			
6	0.00000	20.000	1020.5			
7	10.000	20.000	980.18			
8	20.000	20.000	937.04			
11	50.000	20.000	784.29			

Refprop

Delete current row?

Clicking on a table cell and pressing the delete key will erase the data from that row, but the row itself will remain.

10. MANIPULATING DATA TABLES AND PLOTS
(The Window Menu)

Each table or plot appears in a separate window and can be accessed, rearranged, or retitled with commands in the Window menu. The Window menu contains the three permanent options Tile, Cascade, and Retitle. An additional menu item is provided for each table or plot window on the screen. The number of windows is limited only by available memory.

10.1 Arranging Windows on the Screen

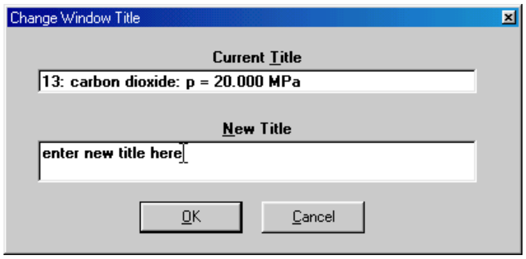
The Tile command resizes and repositions the existing windows so that all are displayed.

The Cascade command overlaps all of the existing windows so that their title bars are visible, making it easy to select any of the windows.

In addition to the Tile and Cascade commands, windows can be rearranged in the usual fashion by clicking and dragging on the title bar. Windows can be resized by clicking and dragging the lower right corner or by using the buttons in the top right corner.

10.2 Retitling Windows

Each table and plot is provided with a default title when it is generated. These titles are used to identify the window(s) acted upon in the Save Tables, Print, New Plot, and Overlay Plot commands. The title of any window can be changed by first clicking anywhere in the window or clicking its title under the Window menu (to make it the active window) and then clicking on the Retitle command. A dialog box appears listing the current title with an edit box where a new title can be entered.



Current Title: 13: carbon dioxide: p = 20.000 MPa

New Title: enter new title here

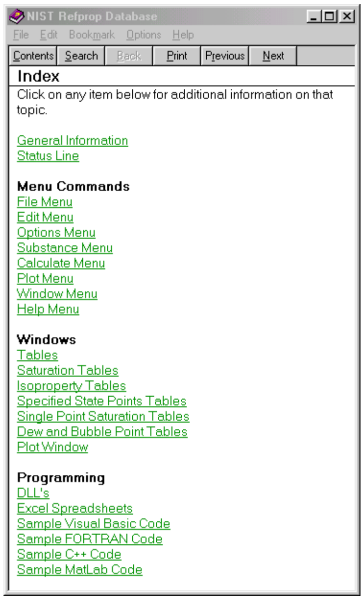
10.3 Going to a Window

Any window on the screen can be brought to the front and made the active window by clicking anywhere in the window. Alternately, you can click its title under the Window menu.

11. THE ON-LINE HELP SYSTEM
(The Help Menu)

On-line help is available under the Help menu. The help system used in REFPROP is a standard implementation and works in the manner of most other Windows applications. Instructions for using the help system are available through the Using Help command.

The Help Index command brings up a listing of the main topics in the help system. Click on the item for which you would like additional information. You can also access Help from most individual dialog boxes. Pressing the F1 key places you in the help system at the point containing instructions for the use of that dialog.



Index

Click on any item below for additional information on that topic.

General Information
Status Line

Menu Commands
File Menu
Edit Menu
Options Menu
Substance Menu
Calculate Menu
Plot Menu
Window Menu
Help Menu

Windows
Tables
Saturation Tables
Isoproperty Tables
Specified State Points Tables
Single Point Saturation Tables
Dew and Bubble Point Tables
Plot Window

Programming
DLL's
Excel Spreadsheets
Sample Visual Basic Code
Sample FORTRAN Code
Sample C++ Code
Sample MatLab Code

A search capability is available by pressing the Search button. The previous topic is recalled by pressing the Back button. The History button (which is accessed from the Help Options menu) lists, and gives you access to, the last several topics viewed.

The About REFPROP command brings up the banner that is displayed on the opening screen.

Appendix A

FLUIDS IN THE REFPROP DATABASE
(Version 7.0)

Short Name	CAS number	Full Chemical Name
ammonia	7664-41-7	ammonia
argon	7440-37-1	argon
butane	106-97-8	butane
carbon dioxide	124-38-9	carbon dioxide
ethane	74-84-0	ethane
isobutane	75-28-5	2–methylpropane
methane	74-82-8	methane
nitrogen	7727-37-9	nitrogen
oxygen	7782-44-7	oxygen
propane	74-98-6	propane
propylene	115-07-1	propene
R11	75-69-4	trichlorofluoromethane
R12	75-71-8	dichlorodifluoromethane
R13	75-72-9	chlorotrifluoromethane
R14	75-73-0	tetrafluoromethane
R22	75-45-6	chlorodifluoromethane
R23	75-46-7	trifluoromethane
R32	75-10-5	difluoromethane
R41	593-53-3	fluoromethane
R113	76-13-1	1,1,2–trichloro–1,2,2–trifluoroethane
R114	76-14-2	1,2–dichloro–1,1,2,2–tetrafluoroethane
R115	76-15-3	chloropentafluoroethane
R116	76-16-4	hexafluoroethane
R123	306-83-2	1,1–dichloro–2,2,2–trifluoroethane
R124	2837-89-0	1–chloro–1,2,2,2–tetrafluoroethane
R125	354-33-6	pentafluoroethane
R134a	811-97-2	1,1,1,2–tetrafluoroethane
R141b	1717-00-6	1,1–dichloro–1–fluoroethane
R142b	75-68-3	1–chloro–1,1–difluoroethane
R143a	420-46-2	1,1,1–trifluoroethane
R152a	75-37-6	1,1-difluoroethane
R218	76-19-4	octafluoropropane
RC318	115-25-3	octafluorocyclobutane
R227ea	431-89-0	1,1,1,2,3,3,3–heptafluoropropane
R236ea	431-63-0	1,1,1,2,3,3–hexafluoropropane
R236fa	690-39-1	1,1,1,3,3,3–hexafluoropropane
R245ca	679-86-7	1,1,2,2,3–pentafluoropropane
R245fa	460-73-11	1,1,1,3,3–pentafluoropropane
water	7732-18-5	water

PREDEFINED MIXTURES IN THE REFPROP DATABASE

ASHRAE Designation	Components	Composition (mass percentages)
air	N2/Ar/O2	75.57/1.27/23.16
R401A	R22/152a/124	53/13/34
R401B	R22/152a/124	61/11/28
R401C	R22/152a/124	33/15/52
R402A	R125/290/22	60/2/38
R402B	R125/290/22	38/2/60
R403A	R290/22/218	5/75/20
R403B	R290/22/218	5/56/39
R404A	R125/143a/134a	44/52/4
R405A	R22/152a/142b/C318	45/7/5.5/42.5
R406A	R22/600a/142b	55/4/41
R407A	R32/125/134a	20/40/40
R407B	R32/125/134a	10/70/20
R407C	R32/125/134a	23/25/52
R407D	R32/125/134a	15/15/70
R407E	R32/125/134a	25/15/60
R408A	R125/143a/22	7/46/47
R409A	R22/124/142b	60/25/15
R409B	R22/124/142b	65/25/10
R410A	R32/125	50/50
R410B	R32/125	45/55
R411A	R1270/22/152a	1.5/87.5/11.0
R411B	R1270/22/152a	3/94/3
R412A	R22/218/142b	70/5/25
R413A	R218/143a/600a	9/88/3
R414B	R22/124/600a/142b	50/39/1.5/9.5
R416A	R22/124/600a/142b	50.0/39.0/1.5/9.5
R417A	R125/134a/600	46.6/50.0/3.4
R500	R12/152a	73.8/26.2
R501	R22/12	75/25

R502	R22/115	48.8/51.2
R503	R23/13	40.1/59.9
R504	R32/115	48.2/51.8
R507A	R125/143a	50/50
R508A	R23/116	39/61
R508B	R23/116	46/54
R509A	R22/218	44/56

Appendix B

PROPERTY MODELS

B.1 Thermodynamic Models

REFPROP calculates the thermodynamic properties using comprehensive equations of state. This approach ensures thermodynamic consistency and allows calculations at all conditions. Other approaches, such as the combination of a vapor-phase model with vapor pressure and liquid density equations may not be applicable in the compressed liquid and supercritical regions and do not always give reliable results for derived properties such as heat capacity and speed of sound.

B.1.1 Pure fluid equations of state

Three models are used for the thermodynamic properties of pure components, depending on the availability of data. The first is the modified Benedict-Webb-Rubin (MBWR) equation of state. This model was first proposed by Jacobsen and Stewart (1973) and has been applied to a wide variety of fluids, including hydrocarbons, cryogenic fluids, and refrigerants. It is capable of accurately representing the properties of a fluid over wide ranges of temperature, pressure, and density. The MBWR equation is the basis for the current international standard for the properties of R123 (Younglove and McLinden, 1994).

The MBWR equation expresses pressure as an explicit function of temperature and molar density and is of the form,

$$P = \sum_{n=1}^{9} \alpha_n \rho^n + exp\left[\left(\rho / \rho^{crit}\right)^2\right] \sum_{n=10}^{15} \alpha_n \rho^{2n-17}, \tag{1}$$

where the a_i are simple functions of temperature resulting in a total of 32 adjustable parameters. For a complete description of the energy quantities (enthalpy, entropy, etc.), the MBWR equation is combined with an expression for the molar heat capacity of the ideal-gas state, that is, vapor in the limit of zero pressure. A form combining polynomial and theoretical terms is used:

$$C_p^{id} = \sum_i c_i T^{ti} + \sum_k \frac{u_k^2 \, exp(u_k)}{\left[exp(u_k) - 1\right]^2} , \tag{2}$$

with

$$u_k = \frac{c_k}{T} . \tag{3}$$

All of the thermodynamic properties can be computed from Eqs. (1–3), as detailed by Younglove and McLinden (1994).

The second high-accuracy pure-fluid equation of state is expressed in terms of reduced molar Helmholtz free energy:

$$a = \frac{A}{RT} = a^{id} + a^r = ln\,\delta + \sum_i \alpha_i \tau^{t_i} + \sum_k \alpha_k \tau^{t_k} \delta^{d_k} \, exp\left(-\gamma \delta^{l_k}\right) , \tag{4}$$

where the first two terms on the right side of Eq. (4) constitute the ideal-gas contribution a^{id}. They are analogous to the combination of the a_1 term in the MBWR equation of state ($a_1 = RT$) and the ideal-gas heat capacity (Eqs. 2 and 3). The second summation is the residual, or real-fluid, contribution a^r. The temperature and density are expressed in the dimensionless variables $\tau = T^*/T$ and $\delta = \rho/\rho^*$, where T^* and ρ^* are reducing parameters which are often, but not always, equal to the critical parameters. The α_i and α_k are numerical coefficients fitted to experimental data, and the exponents t_i, t_k, and d_k are typically determined by a selection algorithm starting with a large bank of terms. The parameter γ is equal to

0 for terms with $l_k = 0$; it is equal to 1 for terms with $l_k \neq 0$. This "Helmholtz-energy model" is the basis for the international standard formulation for R134a (Tillner-Roth and Baehr, 1994).

This model is sometimes termed the "fundamental equation" because it gives a complete description of the thermodynamic properties, as discussed by Tillner-Roth and Baehr (1994), but the MBWR equation of state combined with a C_p^{id} equation is entirely equivalent. The accuracies of these formulations vary, but those for R123 are typical: experimental data are reproduced with average absolute deviations of 0.04% for densities, 0.05% for vapor pressures, and 0.75% for heat capacities.

The third pure-fluid model is the extended corresponding states (ECS) model of Huber and Ely (1994). It is used for fluids with limited experimental data. Simple corresponding states is based on the assumption that different fluids obey, in reduced coordinates, the same intermolecular force law. This assumption leads to the conclusion that, with the appropriate scaling of temperature and density, the reduced residual Helmholtz energies and compressibilities ($Z=p/RT\rho$) of the unknown fluid "j" and a reference fluid "0" (for which an accurate, wide-ranging equation of state is available) are equal:

$$a_j^r\left(T_j, \rho_j\right) = a_0^r\left(T_0, \rho_0\right), \tag{5}$$

and

$$Z_j\left(T_j, \rho_j\right) = Z_0\left(T_0, \rho_0\right). \tag{6}$$

When combined with an expression for the ideal gas heat capacity (such as Eqs. 2 and 3), all other thermodynamic properties can be calculated. The reference fluid is evaluated at a "conformal" temperature and density:

$$T_0 = \frac{T_j}{f_j} = T_j \frac{T_0^{crit}}{T_j^{crit}\theta(T)} \, , \tag{7}$$

and

$$\rho_0 = \rho_j h_j = \rho_j \frac{\rho_0^{crit}}{\rho_j^{crit}} \phi(T). \tag{8}$$

where the multipliers $1/f_j$ and h_j are termed reducing ratios. Simple corresponding states was developed for spherically symmetric molecules, for which the reducing ratios are simple ratios of the critical parameters. The ECS model extends the method to other types of molecules by the introduction of the "shape factors" θ and ϕ. These shape factors are taken here to be functions of temperature and density. The shape factors are fitted to experimental data, typically vapor pressures and saturated liquid densities. The reference fluid is chosen to provide the best fit of the data and is usually chemically similar to the fluid of interest.

B.1.2 Mixture model

The thermodynamic properties of mixtures are calculated with a new model which was developed, in slightly different forms, independently by Tillner-Roth (1993) and Lemmon (1996, 1999). It applies mixing rules to the Helmholtz energy of the mixture components:

$$a_{mix} = \sum_{j=1}^{n}\left[x_j\left(a_j^{id} + a_j^{r}\right) + x_j \ln x_j\right] + \sum_{p=1}^{n-1}\sum_{q=p+1}^{n} x_p x_q F_{pq} a_{pq}^{excess} \tag{9}$$

This mixing formula may be applied directly to the Helmholtz equation of state. Application to the MBWR equation of state and the ideal gas heat capacity expression used with the MBWR and ECS models requires transformations:

$$a^r = \frac{1}{RT}\int_V^\infty (P - RT\rho)\, dV, \tag{10}$$

$$a^{id} = \frac{h_{ref}}{RT} - \frac{S_{ref}}{R} - 1 + \ln\left(\frac{\mathrm{T}\rho}{\mathrm{T}_{ref}\rho_{ref}}\right) + \frac{1}{RT}\int_{T_{ref}}^{T} C_p^{id}\, dT - \frac{1}{R}\int_{T_{ref}}^{T} \frac{C_p^{id}}{T}\, dT \tag{11}$$

where h_{ref} and S_{ref} are an arbitrary reference enthalpy and entropy at the reference state specified by T_{ref} and ϱ_{ref}.

The first summation in Eq. (9) represents the ideal solution; it consists of ideal gas (superscript id) and residual or real fluid (superscript r) terms for each of the pure fluids in the n component mixture. The $x_j \ln x_j$ terms arise from the entropy of mixing of ideal gases where x_j is the mole fraction of component j. The double summation accounts for the “excess” free energy or “departure” from ideal solution. The F_{pq} are generalizing parameters which relate the behavior of one binary pair with another; F_{pq} multiplies the $a_{pq}{}^{excess}$ term(s), which are empirical functions fitted to experimental binary mixture data. The a^r and $a_{pq}{}^{excess}$ functions in Eqs. (9 and 10) are not evaluated at the temperature and density of the mixture T_{mix} and ρ_{mix} but, rather, at a reduced temperature and density τ and δ. These τ and δ are very much in the spirit of the conformal temperature and density of the ECS method and are a key innovation in this model. The mixing rules for the reducing parameters used in REFPROP are:

$$\tau = \frac{T^*}{T_{mix}},\ \text{with}\ T^* = \sum_{p=1}^{n}\sum_{q=1}^{n} k_{T,pq} x_p x_q \frac{1}{2}\left(T_p^{crit} + T_q^{crit}\right),$$

(12)

and

$$\delta = \frac{\rho_{mix}}{\rho^*},\ \text{with}\ \frac{1}{\rho^*} = \sum_{p=1}^{n}\sum_{q=1}^{n} k_{V,pq} x_p x_q \frac{1}{2}\left(\frac{1}{\rho_p^{crit}} + \frac{1}{\rho_q^{crit}}\right).$$

(13)

Equivalent forms which combine the $k_{T,pq}$ with the critical temperatures and the $k_{V,pq}$ with the critical densities are also used:

$$\frac{1}{\rho^*} = \sum_{p=1}^{n} x_p \frac{1}{\rho_p^{crit}} + \sum_{p=1}^{n-1}\sum_{q=p+1}^{n} \xi_{pq} x_p x_q,$$

(14)

and

$$T^* = \sum_{p=1}^{n} x_p T_p^{crit} + \sum_{p=1}^{n-1}\sum_{q=p+1}^{n} \zeta_{pq} x_p^{\beta_{pq}} x_q.$$

(15)

If only limited vapor-liquid equilibrium (VLE) data are available the a_{pq}^{excess} term is taken to be zero, and only the $k_{T,pq}$ and/or $k_{V,pq}$ parameters are fitted. The $k_{T,pq}$ parameter is most closely associated with bubble point pressures, and it is necessary to reproduce azeotropic behavior. The $k_{V,pq}$ parameter is associated with volume changes on mixing. (Ternary and higher order mixtures are modeled in terms of their constituent binary pairs: $k_{T,pq} = 1$ and $k_{V,pq} = 1$ for $p = q$.) If extensive data, including single-phase pressure-volume-temperature (PVT) and heat capacity data, are available, the a_{pq}^{excess} function can be determined. The F_{pq} parameter is used (either alone or in combination with $k_{T,pq}$ and $k_{V,pq}$) to generalize the detailed mixture behavior described by the a_{pq}^{excess} function to other, similar, binary pairs. Lemmon (1996) has determined an a_{pq}^{excess} function based on data for 28 binary pairs of hydrocarbons, inorganics, and HFC's.

This “mixture Helmholtz-energy model” provides a number of advantages. By applying mixing rules to the Helmholtz energy of the mixture components, it allows the use of high-accuracy equations of state for the components, and the properties of the mixture will reduce exactly to the pure components as the composition approaches a mole fraction of unity. Different components in a mixture may be modeled with different forms; for example, a MBWR equation may be mixed with a Helmholtz equation of state. If the components are modeled with the ECS method, this mixture model allows the use of a different reference fluid for each component. The mixture is modeled in a fundamental way, and thus the departure function is generally a relatively small contribution to the total Helmholtz energy for most refrigerant mixtures. The great flexibility of the adjustable parameters in this model allows an accurate representation of a wide variety of mixtures, provided sufficient experimental data are available.

B.2 Mixture Critical Parameters

The reducing temperature and density T* and ρ* in the mixture Helmholtz energy model (Equations 12 – 15) are not the critical parameters for the mixture. The thermodynamic criteria for the critical loci of a binary mixture are

$$\left(\frac{\partial^2 g}{\partial x^2}\right)_{P,T} = 0 \tag{16}$$

and

$$\left(\frac{\partial^3 g}{\partial x^3}\right)_{P,T} = 0 \tag{17}$$

where *g* is the molar Gibbs free energy. The solution of these equations is iterative. Equations (16) and (17) have been solved for selected mixtures and the resulting critical loci have been fitted to empirical functions

$$T^{crit} = x_i T_i^{crit} + x_j T_j^{crit} + \sum_{k=1}^{6} c_k x_i^k x_j \ , \tag{18}$$

where the c_k are fitting parameters; they are stored in the mixture data file and are read upon calling the SETUP subroutine. An analogous function is used for the critical volume. Where these functions are not available, the critical loci are taken to be linear combinations of the pure-component critical parameters (*i.e.* the c_k are all zero).

For three-component and higher-order mixtures, the thermodynamic criteria for the critical loci become increasingly complicated and time consuming to calculate. The number of possible mixture combinations also increases geometrically with the number of components. These factors make it impractical to store critical surfaces for such mixtures. Instead, REFPROP combines the constituent binary critical lines to approximate the critical parameters by

$$T^{crit} = \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} x_i x_j T_{ij}^{crit}(z)}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} x_i x_j} \ , \tag{19}$$

where the $T^{crit}_{ij}(z)$ is the binary critical locus for the binary pair (i,j) evaluated at a pseudo-composition *z*, based on the mixture composition *x*

$$z_i = \frac{x_i + \left(1 - x_j\right)}{2} \tag{20}$$

and

$$z_j = \frac{x_j + \left(1 - x_i\right)}{2} \ , \tag{21}$$

Again, an analogous expression is used to find the critical volume. This method reduces correctly to the pure-component and binary-pair limits, but is otherwise completely empirical. It yields critical parameters which are approximations, and they should be used with caution.

The critical pressure is calculated from the mixture equation of state given the critical temperature and volume computed by the method outlined above.

B.3 Surface Tension Model

The surface tension of pure fluids is modeled as a polynomial in the dimensionless temperature τ

$$\sigma = \sum_{k=0}^{n} \sigma_k \tau^{d_k} \ , \tag{22}$$

where

$$\tau = 1 - \frac{T}{T^{crit}} \ . \tag{23}$$

This form is almost universally used in the literature to represent experimental surface tension data. Often, a summation consisting of a single term, with the exponent on τ equal to approximately 1.26, is sufficient to represent surface tension.

For mixtures, the model of Moldover and Rainwater (1988), as implemented by Holcomb (1997), is used. In this method, the pure fluids are assumed to be correlated with a function of the form

$$\sigma_i = \sigma_{0,i}\tau^{1.26} \ . \tag{24}$$

Although the mixture components may be modeled with a multi-term function, Equation (24) suffices over any limited range of temperature. An "effective" $\sigma_{0,i}$ for each component is computed for the τ of the mixture by using the appropriate pure-fluid model to calculate σ_i. The $\sigma_{0,i}$ and the critical parameters for the pure components yield the C_i, a parameter stemming from the Moldover-Rainwater vapor pressure relationship,

$$C_i = \frac{\sigma_{0,i}^{3/2}}{3.74^{3/2}\left(RT_i^{crit}\right)^{1/2} P_i^{crit}\alpha(1-\alpha)(2-\alpha)} \ , \tag{25}$$

where R is the gas constant and α = 0.1. The effective C for the mixture is given by

$$C_{mix} = \sum_{i=1}^{n} z_i C_i \ , \tag{26}$$

where the z_i is a pseudo-composition based on the fugacity fraction

$$z_i = \frac{f_i}{\sum\limits_{i=1}^{n} f_i} \ . \tag{27}$$

The “effective” σ_0 for the mixture is then recovered by

$$\sigma_{0,mix} = 3.74\left(RT^{crit}\right)^{1/3}\left[C_{mix}P^{crit}\alpha(1-\alpha)(2-\alpha)\right]^{2/3} , \tag{28}$$

and used in Equation (24) to compute the mixture surface tension. The critical temperature and pressure in Equation (28) are evaluated at a mixture composition having the same fugacity fraction at its critical point as the subject mixture at the input *(T,x)*, *i.e.* the z_i given by Equation (27).

B.4 Transport Property Models

The transport properties of viscosity and thermal conductivity are modeled with the residual concept. In this representation, the property Λ (representing either viscosity η or thermal conductivity λ) is composed of several contributions:

$$\Lambda = \Lambda^{id}(T) + \rho\Lambda^{1}(T) + \Lambda^{r}(T,\rho) + \Lambda^{c}(T,\rho) . \tag{29}$$

Λ^{id} is a dilute gas term which is a function only of temperature, Λ^1 accounts for the behavior at moderate densities, and Λ^r is a residual term accounting for the behavior at higher densities, including liquid densities. Λ^r is primarily a function of density, but it may also be a function of both temperature and density.

The initial density dependence Λ^1 follows from the Rainwater-Friend theory (Friend and Rainwater 1984). Although this theory has been developed for both viscosity and thermal conductivity, it is usually applied only to viscosity. The thermal conductivity approaches infinity at the critical point, and this critical enhancement is expressed by Λ^c. This term is significant for thermal conductivity even quite far from the critical point. For viscosity, the enhancement is small except extremely close to the critical point and may be safely ignored in all practical applications.

A variety of models for viscosity and thermal conductivity, based on the residual concept, have been implemented in the database. This section describes, in general terms, the models used. The references listed below or in the pure-fluid information screens in the interface give more details.

B.4.1 Pure fluid viscosity models

We have consolidated a variety of fluid-specific correlations for viscosity into a generalized form. The following equations, and also those for thermal conductivity, are written in terms of a reduced temperature τ and density δ where $\tau = T/T^{red}$ and $\delta = \rho/\rho^{red}$. The viscosity and thermal conductivity also involve reducing parameters η^{red} and λ^{red}. These reducing parameters are used, for example, to convert units, and they may be different for the various terms in each model. The a_k, b_k, d_k, t_k, e_k, l_k, m_k, and n_k are adjustable parameters, and the C represent theoretically based constants.

The dilute-gas contribution is expressed as a combination of the Chapman-Enskog term arising from kinetic theory and an empirical term:

$$\frac{\eta^{id}}{\eta^{red}} = \frac{CM^{1/2}T^{1/2}}{\sigma^2\Omega(T^*)} + \sum a_k \tau^{t_k} \ , \tag{30}$$

where M is the molecular weight, σ is the Lennard-Jones size parameter, and we use the empirical function of Bich *et al.* (1987) to represent the reduced effective collision cross section Ω:

$$\Omega = \exp\left[\sum_{i=0}^{4} b_i \left[\ln(T^*)\right]^i\right] , \tag{31}$$

where $T^* = Tk/\epsilon$ and ϵ/k is the Lennard-Jones energy parameter.

The initial density dependence is given by Friend and Rainwater (1984):

$$\frac{\eta^1}{C\sigma^3} = \sum_{i=0}^{12} b_i \left(\frac{T}{\varepsilon / k} \right)^{-i/2} . \tag{32}$$

The residual term is expressed as a combination of several empirical terms

$$\frac{\eta^r}{\eta^{red}} = \sum a_k \tau^{t_k} \delta^{d_k} \exp\left(-\delta^{l_k}\right) + \frac{\sum a_k \tau^{t_k} \delta^{d_k} \rho_0^{e_k}}{\sum b_k \tau^{t_k} \delta^{d_k} \rho_0^{e_k}} + \exp\left[\frac{\sum a_k \tau^{t_k} \delta^{d_k} \rho_0^{e_k}}{\sum b_k \tau^{t_k} \delta^{d_k} \rho_0^{e_k}} \right] , \tag{33}$$

where the close-packed density ρ_0 is given by

$$\rho_0 = \sum a_k \tau^{t_k} . \tag{34}$$

Equations 30–34 represent, with minor transformations, the viscosity formulations of Laesecke (1997) for R134a, Tanaka (1995) for R123, Fenghour *et al.* (1995) for ammonia, and Krauss *et al.* (1996) for R152a, among others. (Many of the terms are zero for various formulations.) For some of the hydrocarbons, we adopt the fluid-specific formulations of Younglove and Ely (1987). See their paper for a description of this model.

B.4.2 Pure fluid thermal conductivity models

The primary model for thermal conductivity represents the dilute-gas and residual terms as rational polynomials

$$\frac{\lambda^{id}}{\lambda^{red}} = \frac{\sum a_k \tau^{t_k}}{\sum b_k \tau^{t_k}} \tag{35}$$

and

$$\frac{\lambda^{r}}{\lambda^{red}} = \frac{\sum a_k \tau^{t_k} \delta^{d_k}}{\sum b_k \tau^{t_k} \delta^{d_k}} \ . \tag{36}$$

Equations 35 and 36 consolidate into a general form, a variety of fluid-specific correlations, including those of Perkins *et al.* (1998) for R134a, Krauss *et al.* (1996) for R152a, and Laesecke *et al.* (1996) for R123.

The critical enhancement for thermal conductivity is represented using two models. The first is an empirical form used by Laesecke *et al.* (1996):

$$\frac{\lambda^{c}}{\lambda^{red}} = \frac{\sum a_k (m_k + \tau)^{t_k} (n_k + \delta)^{d_k}}{\sum b_k (m_k + \tau)^{t_k} (n_k + \delta)^{d_k}} + \sum \exp\left[a_k (m_k + \tau)^{t_k} (n_k + \delta)^{d_k} \right]. \tag{37}$$

The second critical enhancement model is a theoretical form used by Perkins *et al.* (1998) for R134a, Krauss *et al.* (1996) for R152a, and Vesovic *et al.* (1990) for carbon dioxide. We adopt the “simplified” form of this model, as presented by Olchowy and Sengers (1989); it involves the viscosity η and the isochoric and isobaric heat capacities C_v and C_p

$$\frac{\lambda^c}{\lambda^{red}} = \rho C_p \frac{kR_0T}{6\pi\eta(T,\rho)\xi}\left(\tilde{\Omega} - \tilde{\Omega}_0\right)$$

(38)

where

$$\tilde{\Omega} = \frac{2}{\pi}\left[\left(\frac{C_p - C_\nu}{C_p}\right)\tan^{-1}(\tilde{q}_D\xi) + \frac{C_V}{C_p}\tilde{q}_D\xi\right]$$

(39)

and

$$\tilde{\Omega}_0 = \frac{2}{\pi}\left\{1 - \exp\left[\frac{-1}{(\tilde{q}_D\xi)^{-1} + \frac{1}{3}\left(\tilde{q}_D\xi\rho^{crit}/\rho\right)^2}\right]\right\}.$$

(40)

The correlation length ξ is given by

$$\xi = \xi_0\left[\frac{\tilde{\chi}(T,\rho) - \tilde{\chi}(T_{ref},\rho)\dfrac{T_{ref}}{T}}{\Gamma}\right]^{\nu/\gamma}$$

(41)

where

$$\tilde{\chi}(T,\rho) = \frac{P^{crit}\rho}{\left(\rho^{crit}\right)^2}\left(\frac{\partial\rho}{\partial P}\right)_T .$$

(42)

In Equations 38–42, R_0, υ, and γ are theoretically based constants; q_D, ξ_0, and Γ are fluid-specific (fitted) terms; T_{ref} is an arbitrary reference temperature which is significantly above the critical temperature; and k is Boltzman's constant.

For some of the hydrocarbons, we adopt the fluid-specific formulations (including dilute-gas, residual, and critical-enhancement terms) of Younglove and Ely (1987). See their paper for a description of this model.

B.4.3 Extended corresponding states model for pure fluids

For those pure fluids which do not have wide-ranging, fluid-specific correlations available, REFPROP uses the extended corresponding states (ECS) models of Klein *et al.* (1997) and McLinden and Klein (1998) for viscosity and thermal conductivity, respectively. These models are modifications to the Huber and Ely (1992) and Huber *et al.* (1992) models used in previous versions of REFPROP.

The dilute-gas contributions are given by kinetic theory:

$$\eta^{id}(T) = C\frac{(MT)^{1/2}}{\sigma^2\Omega^{(2,2)}(kT/\varepsilon)} \tag{43}$$

and

$$\lambda^{id}(T) = \frac{f_{int}\eta^{id}(T)}{M}\left[C_p^{id} - \frac{5}{2}R\right] + \frac{15R\eta^{id}(T)}{4M}\ , \tag{44}$$

where we use the empirical function of Neufeld *et al.* (1972) for the collision integral $\Omega^{(2,2)}$, and the f_{int} is fitted as a linear function of temperature (if sufficient data are available) or set to the constant $1.32\text{x}10^{-3}$.

As in the ECS model for the thermodynamic properties, the residual parts of the transport properties are based on those of a reference fluid (R134a for the refrigerants in REFPROP):

$$\eta^r(T,\rho) = \eta_0^r\left(T_0, \rho_{0,\eta}\right) f^{1/2} h^{-2/3} \left(\frac{M}{M_0}\right)^{1/2}$$

(45)

and

$$\lambda^r(T,\rho) = \lambda_0^r\left(T_0, \rho_{0,\lambda}\right) f^{1/2} h^{-2/3} \left(\frac{M_0}{M}\right)^{1/2} .$$

(46)

The conformal temperature T_0 and density ρ_0 are found by solving Equations 5 and 6; these values are then used to find the reducing ratios *f* and *h* by Equations 7 and 8. The conformal densities at which the reference fluid formulations are evaluated are modified from those in the thermodynamic ECS model by additional viscosity and thermal conductivity shape factors

$$\rho_{0,\eta} = \Psi\left(\rho / \rho^{crit}\right) h\rho$$

(47)

and

$$\rho_{0,\lambda} = \chi\left(\rho / \rho^{crit}\right) h\rho ,$$

(48)

where Ψ and χ are empirical polynomials in the reduced density.

The critical enhancement for thermal conductivity is calculated using the method of Olchowy and Sengers (1989).

B.4.4 Extended corresponding states model for mixtures

The transport properties of mixtures are modeled with the extended corresponding states (ECS) models of Klein *et al.* (1997) and McLinden and Klein (1998) for viscosity and thermal conductivity, respectively. These models are modifications to the Huber and Ely (1992) and Huber *et al.* (1992) models used in previous versions of REFPROP.

Mixture transport properties are composed of the same terms present for the pure fluids. The dilute-gas contribution is calculated by matrix analogs of Equations 43 and 44; see, for example, Hirschfelder *et al.* (1967). All quantities in the dilute-gas terms are evaluated at the temperature of the mixture, rather than some conformal temperature.

The residual contribution is found by combining the properties of the reference fluid, evaluated at the conformal conditions given by the solution of:

$$\alpha_0^r\left(T_0, \rho_0\right) = \alpha_{mix}^r(T, \rho, x) \tag{49}$$

and

$$Z_0\left(T_0, \rho_0\right) = Z_{mix}(T, \rho, x) \tag{50}$$

with the viscosity or thermal conductivity of each of the components, evaluated at the conformal conditions given by

$$\alpha_j^r\left(T_j, \rho_j\right) = \alpha_{mix}^r(T, \rho, x) \tag{51}$$

and

$$Z_j\left(T_j, \rho_j\right) = Z_{mix}(T, \rho, x) \tag{52}$$

where the subscripts 0 and *j* refer to the reference fluid and component *j* in the mixture, respectively. The reducing parameters are then defined by

$$f_x = \frac{T}{T_0} \ ,$$ (53)

$$h_x = \frac{\rho_0}{\rho} \ ,$$ (54)

$$f_j = \frac{T_j f_x}{T} \ ,$$ (55)

and

$$h_j = \frac{\rho h_x}{\rho_j} \ .$$ (56)

The ratio of molar masses $(M_0/M)^{1/2}$ in equations 45 and 46 is replaced by

$$g_x^{1/2} = \frac{M_0^{1/2} f_x^{1/2} h_x^{4/3}}{\sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j \left(f_i f_j\right)^{1/2} \left(\frac{2}{1/g_i + 1/g_j}\right)^{1/2} \left[\frac{1}{8}\left(h_i^{1/3} + h_j^{1/3}\right)^3\right]^{4/3}} \ ,$$ (57)

where

$$g_i = M_0 \left[\frac{\Lambda_0^r\left(T_0, \rho_0\right)}{\Lambda_j^r\left(T_j, \rho_j\right)}\right]^2 f_j h_j^{-4/3} \ .$$ (58)

Again, the Λ represents either viscosity or thermal conductivity. Including the pure component values in this way ensures that the properties of a mixture reduce to the pure fluid values as the composition approaches 1.

B.5 References

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Appendix C

USING REFPROP WITH OTHER PROGRAMS
FORTRAN SOURCE CODE

The subroutines are contained in the following files which are placed in the FORTRAN directory by the installation script. They should be compiled and linked with your own main program:

core_ANC.for
core_BWR.for
core_CPP.for
core_DE.for
core_ECS.for
core_FEQ.for
cor_MLT.for
core_PH0.for
core_STN.for
flash2.for
flsh_sub.for
idealgas.for
mix_HMX.for
prop_sub.for
realgas.for
sat_sub.for
setup.for
setup2.for
trnsp.for
trns_ECS.for
trns_TCX.for
trns_VIS.for
utility.for

All the above files are required.

Several additional files are provided. The file “example.for” is a main program providing simple examples of calling the property routines. The file “pass_ftn.for” contains the interface routines used by the graphical interface and dynamic link libraries; the file ftn_pas.for is similar and is included for compatibility with Version 6. They would not be needed by ordinary FORTRAN applications. The file “X_sub.for” contains alternative versions of the most commonly called REFPROP routines. These routines are the same as the standard ones except that they have only integer and real arguments (no character strings) and so are intented for cross-language applications that cannot handle strings conveniently (e.g., LabView).

Any fluids which are used must have a corresponding “.fld” file, *e.g.* R134a.fld or propane.fld. The file “HMX.bnc” (containing mixture parameters) must also be present. It is suggested (but not required) that these be put into a subdirectory called “fluids” under the directory containing the application program.

The subroutine SETUP must be called to initialize the pure fluid or mixture components. The call to SETUP will allow the choice of one of several standard reference states for entropy and enthalpy and will automatically load the “NIST-recommended” models for the components as well as mixing rules. The subroutine SETMOD allows the specification of other models. The subroutine SETKTV allows the specification of mixing rules and parameters. To define another reference state, or to apply one of the standard states to a mixture of a specified composition, the subroutine SETREF may be used. These subroutines should be called only if the fluids and/or models (or reference state) are changed.

The sequence is:

call SETMOD	(optional)
call SETUP	(REQUIRED)
call SETKTV	(optional)
call SETREF	(optional)

C.1 Units

All inputs and outputs to the subroutines are in the following units:

temperature	K
pressure, fugacity	kPa
density	mol/L
composition	mole fraction
quality	mole basis
(except mass basis allowed when quality is input)	
enthalpy, internal energy	J/mol
Gibbs, Helmholtz free energy	J/mol
entropy, heat capacity	J/(mol·K)
speed of sound	m/s
Joule-Thompson coefficient	K/kPa
d(p)/d(rho)	kPa·L/mol
$d^2(p)/d(rho)^2$	$kPa\cdot(L/mol)^2$
viscosity	μPa·s (10^{-6} Pa·s)

thermal conductivity	W/(m·K)
dipole moment	debye
surface tension	N/m

C.2 Naming conventions

The variable type of subroutine arguments can generally be inferred from the first letter of the variable name:

a-g and o-z:	double precision
h:	double precision (*i.e.* enthalpy) or character
i-k and m,n:	integer
l:	logical (within subroutines only, no logicals are used in arguments) also used as integer for exponent of FEQ model

The property subroutines are compatible with FORTRAN 90. The routines are largely compatible with ANSI standard FORTRAN 77; the only extension widely used is the “do -- enddo” construct, which is supported by most FORTRAN 77 compilers. We have tested the source code on the following compilers:

Absoft Pro FORTRAN 5.0
Digital Visual FORTRAN 5.0
Fortner Research FORTRAN (Macintosh)
Lahey FORTRAN77
Lahey FORTRAN90
Lahey/Fujitsu LF95
Microsoft FORTRAN 5.1
Microsoft PowerStation FORTRAN 4.0

We are striving to make these subroutines as standard and portable as possible, but every compiler has its own sensitive points. Please report any compiler or linker errors or warnings.

Potential pitfalls:

The fluid data files are read using logical unit 12. Use of this unit in your application program may crash the application program and/or the subroutines and should be avoided.

Following is a description of the high-level subroutines that would be used in stand-alone applications. These subroutines will give access to all features in a model-independent fashion. (There are corresponding low-level subroutines for some of these which call specific models. Please do not incorporate the low-level subroutines into your applications—if you do, you may find that future versions may not work the same.)

C.3 Initialization Subroutines

```
      subroutine SETUP (nc,hfiles,hfmix,hrf,ierr,herr)
c
c  define models and initialize arrays
c
c  A call to this routine is required.
c
c  inputs:
c       nc--number of components (1 for pure fluid) [integer]
c     hfiles--array of file names specifying fluid/mixture
components
c               [character*255 variable] for each of the nc
components;
c           e.g., :fluids:R134a.fld (Mac) or fluids\R134a.fld
(DOS) or
c           [full_path]/fluids/R134a.fld (UNIX)
c    hfmix--mixture coefficients [character*255]
c             file name containing coefficients for mixture
model,
c           e.g.,  :fluids:HMX.bnc
c        hrf--reference state for thermodynamic calculations
[character*3]
c             'DEF':  default reference state as specified in
fluid file
c                   is applied to each pure component
c             'NBP':  h,s = 0 at pure component normal boiling
point(s)
c             'ASH':  h,s = 0 for sat liquid at -40 C (ASHRAE
convention)
c             'IIR':  h = 200, s = 1.0 for sat liq at 0 C (IIR
convention)
c             other choices are possible, but these require a
separate
c           call to SETREF
```

```
c  outputs:
c     ierr--error flag:  0 = successful
c                      101 = error in opening file
c                        102 = error in file or premature end
of file
c                         -103 = unknown model encountered in
file
```

```
c                      104 = error in setup of model
c                      105 = specified model not found
c                      111 = error in opening mixture file
c                      112 = mixture file of wrong type
c     herr--error string (character*255 variable if ierr<>0)
c       [fluid parameters, etc. returned via various common
blocks]
      subroutine SETMOD (nc,htype,hmix,hcomp,ierr,herr)
c
c  set model(s) other than the NIST-recommended ('NBS') ones
c
c  This subroutine must be called before SETUP; it need not
be called
c   at all if the default (NIST-recommended) models are
desired.
c
c  inputs:
c       nc--number of components (1 for pure fluid) [integer]
c       htype--flag indicating which models are to be set
[character*3]
c                'EOS':  equation of state for thermodynamic
properties
c           'ETA':  viscosity
c           'TCX':  thermal conductivity
c           'STN':  surface tension
c             'NBS':  reset all of the above model types and
all
c                   subsidiary component models to 'NBS';
c                   values of hmix and hcomp are ignored
c      hmix--mixture model to use for the property specified
in the
c           argument htype [character*3];
c                this can a pure fluid model if number of
components = 1
c              'NBS':  use NIST recommendation for specified
fluid/mixture
c                    (valid input for all properties, pure or
mix)
c
c                  some allowable choices for thermodynamic
properties:
c           pure fluids:
c           'FEQ':  Helmholtz free energy model
c            'BWR':  pure fluid modified Bennedict-Webb-Rubin
(MBWR)
c            'ECS':  pure fluid thermo extended corresponding
states
c           mixture:
c           'HMX':  mixture Helmholtz model for thermodynamic
properties
c
c           some allowable choices for viscosity:
c           pure fluids:
```

```
c                 'ECS':   extended  corresponding  states  (all
fluids)
c             'VS1':  the 'composite' model for R134a, R152a,
NH3, etc.
c           'VS2':  Younglove-Ely model for hydrocarbons
c           mixture:
c           'ECS':  extended corresponding states
c
c           some allowable choices for thermal conductivity:
c           pure fluids:
```

```
c                 'ECS':   extended corresponding states  (all
fluids)
c             'TC1':  the 'composite' model for R134a, R152a,
etc.
c           'TC2':  Younglove-Ely model for hydrocarbons
c           mixture:
c           'ECS':  extended corresponding states
c
c           some allowable choices for surface tension:
c           pure fluids:
c           'ST1':  surface tension as f(tau); tau = 1 - T/Tc
c           mixture:
c           'STX':  surface tension mixture model
c
c     hcomp--component model(s) to use for property specified
in htype
c           [array (1..nc) of character*3]
c                 'NBS':   NIST  recommendation  for  specified
fluid/mixture
c                     (valid input for all properties, pure or
mix)
c                      other choices are identical to the pure
fluid
c                   choices listed above
c  outputs:
c     ierr--error flag:  0 = successful
c                            no errors are returned from this
routine,
c                          ierr and herr included to maintain
parallel
c                           structure and for possible future
use
c     herr--error string (character*255 variable if ierr<>0)
c       [fluid parameters, etc. returned via various  common
blocks]
      subroutine                                       SETKTV
(icomp,jcomp,hmodij,fij,hfmix,ierr,herr)
c
c  set mixture model and/or parameters
c
c  This subroutine must be called after SETUP, but before any
call to
c   SETREF; it  need  not  be  called  at  all  if  the  default
mixture
c  parameters (those read in by SETUP) are to be used.
c
c  inputs:
c    icomp--component i
c    jcomp--component j
c   hmodij--mixing rule for the binary pair i,j [character*3]
c           e.g. 'LJ1' (Lemmon-Jacobsen model) or
c                'LIN' (linear mixing rules)
c                ‘LM1’ (modified Lemmon-Jacobson model)
c           'RST' indicates reset all pairs to values from
```

```
c                     original call to SETUP (i.e. those read
from file)
c                  [all other inputs are ignored]
c         fij--binary mixture parameters [array of dimension
nmxpar;
c           currently nmxpar is set to 6]
c           the parameters will vary depending on hmodij;
c           for example, for the Lemmon-Jacobsen model (LJ1):
c             fij(1) = zeta
```

```
c             fij(2) = xi
c             fij(3) = Fpq
c             fij(4) = beta
c             fij(5) = gamma
c             fij(6) = 'not used'
c     hfmix--file name [character*80] containing generalized
parameters
c             for the binary mixture model; this will usually
be the same
c                     as  the  corresponding  input  to  SETUP
(e.g.,’:fluids:HMX.bnc')
c  outputs:
c     ierr--error flag:  0 = successful
c                        111 = error in opening mixture file
c                        112 = mixture file of wrong type
c                       -113 = illegal i,j specification
c                              (i = j or i > nc or j > nc)
c     herr--error string (character*255 variable if ierr<>0)
c     [mixture parameters returned via various common blocks]
      subroutine SETREF (hrf,ixflag,x0,h0,s0,t0,p0,ierr,herr)
c
c  set reference state enthalpy and entropy
c
c  This subroutine must be called after SETUP; it need not be
called at
c  all if the reference state specified in the call to SETUP
is to be
c  used.
c
c  inputs:
c        hrf--reference  state  for  thermodynamic  calculations
[character*3]
c           'NBP':  h,s = 0 at normal boiling point(s)
c             'ASH':  h,s  =  0  for  sat  liquid  at  -40  C  (ASHRAE
convention)
c            'IIR':  h = 200, s = 1.0 for sat liq at 0 C (IIR
convention)
c             'DEF':  default  reference  state  as  specified  in
fluid file
c                    is applied to each component (ixflag = 1
is used)
c           'OTH':  other, as specified by h0, s0, t0, p0
c   ixflag--composition flag:  1 = ref state applied to pure
components
c                                    2  =  ref  state  applied  to
mixture x0
c  following input has meaning only if ixflag = 2
c         x0--composition  for  which  h0,  s0  apply;  array(1:nc)
[mol frac]
c               this  is  useful  for  mixtures  of  a  predefined
composition,
c           e.g. refrigerant blends such as R410A
c  following inputs have meaning only if hrf = 'OTH'
c       h0--reference state enthalpy at t0,p0 {x0} [J/mol]
```

```
c       s0--reference state entropy at t0,p0 {x0} [J/mol-K]
c       t0--reference state temperature [K]
c              t0 = -1 indicates saturated liquid at normal
boiling point
c                   (bubble point for a mixture)
c       p0--reference state pressure [kPa]
c           p0 = -1 indicates saturated liquid at t0 {and x0}
c           p0 = -2 indicates saturated vapor at t0 {and x0}
c  outputs:
```

```
c     ierr--error flag:  0 = successful
c                         22 = Tmin > Tref for IIR reference
state
c                        23 = Tcrit < Tref for IIR reference
state
c                      24 = Tmin > Tref for ASHRAE reference
state
c                               25 = Tcrit < Tref for ASHRAE
reference state
c                         26 = Tmin > Tnbp for NBP reference
state
c                          27 = Tref, Pref for OTH ref state
outside limits
c                    -28 = can't apply 'DEF' to mixture;
c                            will apply to pure components
c                              -29 = unknown reference state
specified;
c                            will use 'DEF'
c     herr--error string (character*255 variable if ierr<>0)
c       [fluid parameters, etc. returned via various common
blocks]
      subroutine                                       GETKTV
(icomp,jcomp,hmodij,fij,hfmix,hfij,hbinp,hmxrul)
c
c  retrieve mixture model and parameter info for a specified
binary
c
c  This subroutine should not be called until after a call to
SETUP.
c
c  inputs:
c    icomp--component i
c    jcomp--component j
c  outputs:
c   hmodij--mixing rule for the binary pair i,j (e.g. LJ1 or
LIN)
c           [character*3]
c        fij--binary mixture parameters [array of dimension
nmxpar;
c              currently nmxpar is set to 6]; the parameters
will vary
c           depending on hmodij;
c     hfmix--file name [character*255] containing parameters
for the
c           binary mixture model
c       hfij--description of the binary mixture parameters
[character*8
c           array of dimension nmxpar]
c           for example, for the Lemmon-Jacobsen model (LJ1):
c             fij(1) = zeta
c             fij(2) = xi
c             fij(3) = Fpq
c             fij(4) = beta
c             fij(5) = gamma
```

```
c             fij(6) = 'not used'
c         hbinp--documentation  for  the  binary  parameters
[character*255]
c           terminated with ASCII null character
c   hmxrul--description of the mixing rule [character*255]
```

C.4 Saturation-State Subroutines

```
      subroutine                                          SATT
(t,x,kph,p,rhol,rhov,xliq,xvap,ierr,herr)
c
c   iterate for saturated liquid and vapor states given
temperature
c  and the composition of one phase
c
c  inputs:
c        t--temperature [K]
c         x--composition [array of mol frac] (phase specified
by kph)
c        kph--phase flag: 1 = input x is liquid composition
(bubble point)
c                       2 = input x is vapor composition (dew
point)
c                        3 = input x is liquid comp (freezing
point)
c                                4 = input x is vapor comp
(sublimation point)
c  outputs:
c        p--pressure [kPa]
c     rhol--molar density [mol/L] of saturated liquid
c     rhov--molar density [mol/L] of saturated vapor
c     xliq--liquid phase composition [array of mol frac]
c     xvap--vapor phase composition [array of mol frac]
c     ierr--error flag:   0 = successful
c                         1 = T < Tmin
c                         8 = x out of range
c                         9 = T and x out of range
c                       120 = CRITP did not converge
c                       121 = T > Tcrit
c                         122 = TPRHO-liquid did not converge
(pure fluid)
c                          123 = TPRHO-vapor did not converge
(pure fluid)
c                          124 = pure fluid iteration did not
converge
c            following 3 error codes are advisory--iteration
will either
c          converge on later guess or error out (ierr = 128)
c                          -125 = TPRHO did not converge for
parent ph (mix)
c                          -126 = TPRHO did not converge for
incipient (mix)
c                        -127 = composition iteration did not
converge
c                            128 = mixture iteration did not
converge
c     herr--error string if ierr<>0 (character*255)
      subroutine                                          SATP
(p,x,kph,t,rhol,rhov,xliq,xvap,ierr,herr)
c
```

```
c   iterate  for  saturated  liquid  and  vapor  states  given
temperature
c  and the composition of one phase
c
c  inputs:
c        p--pressure [kPa]
c         x--composition [array of mol frac] (phase specified
by kph)
c      kph--phase flag:  1 = input x is liquid composition
c                        2 = input x is vapor composition
c
```

```
c  outputs:
c        t--temperature [K]
c     rhol--molar density [mol/L] of saturated liquid
c     rhov--molar density [mol/L] of saturated vapor
c     xliq--liquid phase composition [array of mol frac]
c     xvap--vapor phase composition [array of mol frac]
c     ierr--error flag:  0 = successful
c                        4 = P < 0
c                        8 = x out of range
c                       12 = P and x out of range
c                      140 = CRITP did not converge
c                      141 = P > Pcrit
c                         142 = TPRHO-liquid did not converge
(pure fluid)
c                          143 = TPRHO-vapor did not converge
(pure fluid)
c                          144 = pure fluid iteration did not
converge
c             following 3 error codes are advisory--iteration
will either
c           converge on later guess or error out (ierr = 148)
c                        -144 = Raoult's law (mixture intial
guess) did
c                             not converge
c                           -145 = TPRHO did not converge for
parent ph (mix)
c                           -146 = TPRHO did not converge for
incipient (mix)
c                         -147 = composition iteration did not
converge
c                             148 = mixture iteration did not
converge
c     herr--error string if ierr<>0 (character*255)
      subroutine                                          SATD
(rho,x,kph,kr,t,p,rhol,rhov,xliq,xvap,ierr,herr)
c
c  iterate for temperature and pressure given a density along
the
c  saturation boundary and the composition
c
c  inputs:
c       rho--molar density [mol/L]
c        x--composition [array of mol frac]
c         kph--flag specifying desired root for multi-valued
inputs
c            has meaning only for water at temps close to its
triple point
c           -1 = return middle root (between 0 and 4 C)
c            1 = return highest temperature root (above 4 C)
c                 3 = return lowest temperature root (along
freezing line)
c  outputs:
c        t--temperature [K]
c        p--pressure [kPa]
```

```
c     rhol--molar density [mol/L] of saturated liquid
c     rhov--molar density [mol/L] of saturated vapor
c     xliq--liquid phase composition [array of mol frac]
c     xvap--vapor phase composition [array of mol frac]
c       kr--phase flag: 1 = input state is liquid
c                               2 = input state is vapor in
equilibrium with liq
c                       3 = input state is liq in equilibrium
with solid
```

```
c                        4 = input state is vap in equilibrium
with solid
c     ierr--error flag:   0 = successful
c                         2 = D > Dmax
c                         8 = x out of range
c                        10 = D and x out of range
c                       160 = CRITP did not converge
c                       161 = SATD did not converge
c     herr--error string (character*255 variable if ierr<>0)
c
c  N.B. kr = 3,4 presently working only for pure components
c
c  either (rhol,xliq) or (rhov,xvap) will correspond to the
input state
c  with the other pair corresponding to the other phase in
equilibrium
c  with the input state
      subroutine                                          SATH
(h,x,kph,nroot,k1,t1,p1,d1,k2,t2,p2,d2,ierr,herr)
c
c  iterate for temperature, pressure, and density given an
enthalpy along
c  the saturation boundary and the composition
c
c  inputs:
c        h--molar enthalpy [J/mol]
c        x--composition [array of mol frac]
c      kph--flag specifying desired root
c           0 = return all roots along the liquid-vapor line
c           1 = return only liquid VLE root
c           2 = return only vapor VLE roots
c           3 = return liquid SLE root (melting line)
c           4 = return vapor SVE root (sublimation line)
c  outputs:
c     nroot--number of roots.  Set to one for kph=1,3,4 if
ierr=0
c        k1--phase of first root (1-liquid, 2-vapor, 3-melt,
4-subl)
c       t1--temperature of first root [K]
c       p1--pressure of first root [kPa]
c       d1--molar density of first root [mol/L]
c        k2--phase of second root (1-liquid, 2-vapor, 3-melt,
4-subl)
c       t2--temperature of second root [K]
c       p2--pressure of second root [kPa]
c       d2--molar density of second root [mol/L]
c     ierr--error flag:   0 = successful
c                         2 = h < hmin
c                         4 = h > hmax
c                         8 = h > htrp (for subl input)
c                       160 = CRITP did not converge
c                         161 = SATH did not converge for one
root
```

```
c                          162 = SATH did not converge for both
roots
c     herr--error string (character*255 variable if ierr<>0)
c
```

```
c  The second root is always set as the root in the vapor at
temperatures
c  below the maximum enthalpy on the vapor saturation line.
If kph = 2,
c  and only one root is found in the vapor (this occurs when
h<hcrit)
c  the state point will be placed in k2,t2,p2,d2.  If kph = 0
and this
c  situation occured, the first root (k1,t1,p1,d1) would be
in the liquid
c  (k1 =1, k2 = 2).
c
c  N.B. kph = 3,4 presently working only for pure components
      subroutine SATS (s,x,kph,nroot,k1,t1,p1,d1,k2,t2,p2,d2,
     &                 k3,t3,p3,d3,ierr,herr)
c
c  iterate for temperature, pressure, and density given an
entropy along
c  the saturation boundary and the composition
c
c  inputs:
c        s--molar entropy [J/mol-K]
c        x--composition [array of mol frac]
c      kph--flag specifying desired root
c           0 = return all roots along the liquid-vapor line
c           1 = return only liquid VLE root
c           2 = return only vapor VLE roots
c           3 = return liquid SLE root (melting line)
c           4 = return vapor SVE root (sublimation line)
c  outputs:
c    nroot--number of roots.  Set to one for kph=1,3,4 if
ierr=0
c       k1--phase of first root (1-liquid, 2-vapor, 3-melt,
4-subl)
c       t1--temperature of first root [K]
c       p1--pressure of first root [kPa]
c       d1--molar density of first root [mol/L]
c       k2--phase of second root (1-liquid, 2-vapor, 3-melt,
4-subl)
c       t2--temperature of second root [K]
c       p2--pressure of second root [kPa]
c       d2--molar density of second root [mol/L]
c       k3--phase of thrid root (1-liquid, 2-vapor, 3-melt,
4-subl)
c       t3--temperature of third root [K]
c       p3--pressure of third root [kPa]
c       d3--molar density of third root [mol/L]
c     ierr--error flag:   0 = successful
c                         2 = s < smin
c                         4 = s > smax
c                         8 = s > strp (for subl input)
c                       160 = CRITP did not converge
c                         161 = SATS did not converge for one
root
```

```
c                         162 = SATS did not converge for two
roots
c                         163 = SATS did not converge for all
roots
```

```
c     herr--error string (character*255 variable if ierr<>0)
c
c  The second root is always set as the root in the vapor at temperatures
c  below the maximum entropy on the vapor saturation line. If kph = 2,
c  and only one root is found in the vapor (this occurs when s<scrit)
c  the state point will be placed in k2,t2,p2,d2.  If kph = 0 and this
c  situation occured, the first root (k1,t1,p1,d1) would be in the liquid
c  (k1=1, k2=2).
c
c  The third root is the root with the lowest temperature.
c  For fluids with multiple roots:  When only one root is found in the
c  vapor phase (this happens only at very low temperatures past the
c  region where three roots are located), the value of the root is still
c  placed in k3,t3,p3,d3.  For fluids that never have more than one root
c   (when there is no maximum entropy along the saturated vapor line), the
c  value of the root is always placed in k1,t1,p1,d1.
c
c  N.B. kph = 3,4 presently working only for pure components
```

```
      subroutine CSATK (icomp,t,kph,p,rho,csat,ierr,herr)
c
c  compute the heat capacity along the saturation line as a function of
c  temperature for a given component
c
c  csat can be calculated two different ways:
c     Csat = Cp - T(DvDT)(DPDTsat)
c     Csat = Cp - beta/rho*hvap/(vliq - vvap)
c     where beta is the volulme expansivity
c
c  inputs:
c     icomp--component number in mixture (1..nc); 1 for pure fluid
c        t--temperature [K]
c      kph--phase flag: 1 = liquid calculation
c                       2 = vapor calculation
c  outputs:
c        p--saturation pressure [kPa]
c      rho--saturation molar density [mol/L]
c     csat--saturation heat capacity [J/mol-K]
```

Two similar routines are provided for calculating surface tension. SURTEN is more efficient if the liquid and vapor density and composition are known (e.g. from a previous call to SATT). If these are not known, then SURFT may be used.

```
      subroutine SURFT (t,rhol,xl,sigma,ierr,herr)
c
c  compute surface tension
c
c  inputs:
c        t--temperature [K]
c       xl--composition of liquid phase [array of mol frac]
c  outputs:
c     rhol--molar density of liquid phase [mol/L]
c    sigma--surface tension [N/m]
c     ierr--error flag:   0 = successful
c                         1 = T < Tmin
c                         8 = x out of range
c                         9 = T and x out of range
c                       120 = CRITP did not converge
c                       121 = T > Tcrit
c                         122 = TPRHO-liquid did not converge
in SATT
c                        123 = TPRHO-vapor did not converge in
SATT
c                         124 = SATT pure fluid iteration did
not converge
c                        128 = SATT mixture iteration did not
converge
c     herr--error string if ierr<>0 (character*255)
```

```
      subroutine SURTEN (t,rhol,rhov,xl,xv,sigma,ierr,herr)
c
c  compute surface tension
c
c  inputs:
c        t--temperature [K]
c     rhol--molar density of liquid phase [mol/L]
c     rhov--molar density of vapor phase [mol/L]
c              if either rhol or rhov < 0 call SATT to find
densities
c       xl--composition of liquid phase [array of mol frac]
c       xv--composition of liquid phase [array of mol frac]
c           (xv is optional input if rhol < 0 or rhov < 0)
c  outputs:
c    sigma--surface tension [N/m]
c     ierr--error flag:   0 = successful
c                          [all error codes identical to those
for SURFT]
c     herr--error string if ierr<>0 (character*255)
```

C.5 Flash Subroutines

So-called “flash” calculations involve a determination of the thermodynamic state given two independent variables plus composition. In addition to the inputs of temperature and pressure which is the most common flash calculation, REFPROP provides routines for virtually all combinations of temperature, pressure, or density as the first variable and density, internal energy, enthalpy, entropy, or quality as the second variable. The combination of enthalpy and entropy is also supported.

Flash subroutines are provided for cases where the state is known to be single phase (liquid or vapor), known to be two-phase (liquid plus vapor), and also for the general case where the phase is not known. Because of the many combinations and their parallel structure, these routines are described in groups. The first two letters of the subroutine name indicate the independent variables, where

```
T = temperature [K]
P = pressure [kPa]
D = density [mol/L]
E = internal energy [J/mol]
H = enthalpy [J/mol]
S = entropy [J/mol-K]
Q = vapor quality [moles vapor/total moles]
    or [kg vapor/total kg] depending on the
    value of the input flag kq
```

C.5.1 General flash subroutines

For cases where the phase is not known, the following routines are available.

```
      subroutine                                         TPFLSH
(t,p,z,D,Dl,Dv,x,y,q,e,h,s,cv,cp,w,ierr,herr)
      subroutine                                         TDFLSH
(t,D,z,p,Dl,Dv,x,y,q,e,h,s,cv,cp,w,ierr,herr)
      subroutine                                         TEFLSH
(t,e,z,kr,p,D,Dl,Dv,x,y,q,h,s,cv,cp,w,ierr,herr)
      subroutine                                         THFLSH
(t,h,z,kr,p,D,Dl,Dv,x,y,q,e,s,cv,cp,w,ierr,herr)
      subroutine                                         TSFLSH
(t,s,z,kr,p,D,Dl,Dv,x,y,q,e,h,cv,cp,w,ierr,herr)
```

```
      subroutine                                        PDFLSH
(p,D,z,t,Dl,Dv,x,y,q,e,h,s,cv,cp,w,ierr,herr)
      subroutine                                        PEFLSH
(p,e,z,t,D,Dl,Dv,x,y,q,h,s,cv,cp,w,ierr,herr)
      subroutine                                        PHFLSH
(p,h,z,t,D,Dl,Dv,x,y,q,e,s,cv,cp,w,ierr,herr)
      subroutine                                        PSFLSH
(p,s,z,t,D,Dl,Dv,x,y,q,e,h,cv,cp,w,ierr,herr)
      subroutine                                        DHFLSH
(D,h,z,t,p,Dl,Dv,x,y,q,e,s,cv,cp,w,ierr,herr)
      subroutine                                        DSFLSH
(D,s,z,t,p,Dl,Dv,x,y,q,e,h,cv,cp,w,ierr,herr)
      subroutine                                        DEFLSH
(D,e,z,t,p,Dl,Dv,x,y,q,h,s,cv,cp,w,ierr,herr)
      subroutine                                        HSFLSH
(h,s,z,t,p,D,Dl,Dv,x,y,q,e,cv,cp,w,ierr,herr)
      subroutine                                        TQFLSH
(t,q,z,kq,p,D,Dl,Dv,x,y,e,h,s,cv,cp,w,ierr,herr)
      subroutine                                        PQFLSH
(p,q,z,kq,t,D,Dl,Dv,x,y,e,h,s,cv,cp,w,ierr,herr)
c
c  flash calculation given two independent variables and bulk
composition
c
c   These routines accept both single-phase and two-phase
states as the
c  input; if the phase is known, the specialized routines are
faster
c
c  inputs--two of the following as indicated by the first two
letters of
c          the subroutine name:
c        t--temperature [K]
c        p--pressure [kPa]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]
c        q--vapor quality [basis specified by kq]
c           q = 0 indicates saturated liquid
c           q = 1 indicates saturated vapor
c           q < 0 or q > 1 are not allowed and will result in
warning

c  additional input--required for all routines
c        z--overall (bulk) composition [array of mol frac]

c  additional input--only for TQFLSH and PQFLSH
c       kq--flag specifying units for input quality
c            kq = 1 quality on MOLAR basis [moles vapor/total
moles]
c             kq = 2 quality on MASS basis [mass vapor/total
mass]
c
```

```
c   outputs--one, two, or all of the following, depending on
the inputs:
c        t--temperature [K]
c        p--pressure [kPa]
c        D--overall (bulk) molar density [mol/L]
c
c  additional outputs--common to all routines
c       Dl--molar density [mol/L] of the liquid phase
c       Dv--molar density [mol/L] of the vapor phase
c           if only one phase is present, Dl = Dv = D
c        x--composition of liquid phase [array of mol frac]
```

```
c        y--composition of vapor phase [array of mol frac]
c           if only one phase is present, x = y = z
c
c   additional  output--common  to  all  routines  except  TQFLSH
and PQFLSH
c        q--vapor quality on a MOLAR basis [moles vapor/total
moles]
c           q < 0 indicates subcooled (compressed) liquid
c           q = 0 indicates saturated liquid
c           q = 1 indicates saturated vapor
c           q > 1 indicates superheated vapor
c               q  =  998  superheated  vapor,  but  quality  not
defined (t > Tc)
c             q  =  999  indicates  supercritical  state  (t  >  Tc)
and (p > Pc)
c
c   additional  outputs--common  to  all  routines,  except  that
input
c                      quantities are not repeated
c        e--overall (bulk) internal energy [J/mol]
c        h--overall (bulk) enthalpy [J/mol]
c        s--overall (bulk) entropy [J/mol-K]
c       Cv--isochoric (constant V) heat capacity [J/mol-K]
c       Cp--isobaric (constant p) heat capacity [J/mol-K]
c        w--speed of sound [m/s]
c           Cp, w are not defined for 2-phase states
c           in such cases, a flag = -9.99998d6 is returned
c     ierr--error flag:  0 = successful
c                        1 = Tin < Tmin
c                        4 = Pin < 0
c                        5 = T and P out of range
c                        8 = x out of range (component and/or
sum < 0
c                            or > 1)
c                        9 = x and T out of range
c                       12 = x out of range and P < 0
c                       13 = x and T and P out of range
c     herr--error string (character*255 variable if ierr<>0)
```

C.5.2 Single-phase flash subroutines

These routines accept only single-phase states as inputs. They will be faster than the corresponding general routines, but will fail if called with an incorrect phase specification. The phase-specific subroutines also do not check limits, so may fail if called outside the range of the equation of state. The following single-phase routines are available.

```
      subroutine TEFL1 (t,e,z,Dmin,Dmax,D,ierr,herr)
      subroutine THFL1 (t,h,z,Dmin,Dmax,D,ierr,herr)
      subroutine TSFL1 (t,s,z,Dmin,Dmax,D,ierr,herr)
```

```
subroutine HSFL1 (h,s,z,Dmin,Dmax,t,D,ierr,herr)
```

```
c
c  inputs--two of the following as indicated by the first two
letters of c          the subroutine name:
c        t--temperature [K]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]

c  additional inputs--required for all routines
c        z--overall (bulk) composition [array of mol frac]
c     Dmin--lower bound on density [mol/L]
c     Dmax--upper bound on density [mol/L]
c
c  outputs:
c        t--temperature [K] (present only for HSFL1)
c        D--molar density [mol/L]
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
```

Single-phase flash routines (continued)

```
      subroutine PEFL1 (p,e,z,kph,t,D,ierr,herr)
      subroutine PHFL1 (p,h,z,kph,t,D,ierr,herr)
      subroutine PSFL1 (p,s,z,kph,t,D,ierr,herr)
c
c  inputs--two of the following as indicated by the first two
letters of
c          the subroutine name:
c        p--pressure [kPa]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]

c  additional inputs--required for all routines
c        z--overall (bulk) composition [array of mol frac]
c      kph--phase flag:  1 = liquid
c                        2 = vapor
c
c  outputs:
c        t--temperature [K]
c        D--molar density [mol/L]
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
```

```
      subroutine DEFL1 (D,e,z,t,ierr,herr)
      subroutine DHFL1 (D,h,z,t,ierr,herr)
      subroutine DSFL1 (D,s,z,t,ierr,herr)
      subroutine PDFL1 (p,D,z,t,ierr,herr)
c
c  inputs--two of the following as indicated by the first two
letters of
c          the subroutine name:
c        p--pressure [kPa]
c        D--density [mol/L]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]

c  additional inputs--required for all routines
c        z--overall (bulk) composition [array of mol frac]
c
c  outputs:
c        t--temperature [K]
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
```

The single-phase temperature-pressure flash is called many times by other routines and has been optimized for speed and requires a specific calling sequence.

```
      subroutine TPRHO (t,p,x,kph,kguess,rho,ierr,herr)
c
c    iterate   for  density   as   a   function   of   temperature,
pressure, and
c  composition for a specified phase
c
c  inputs:
c        t--temperature [K]
c        p--pressure [kPa]
c        x--composition [array of mol frac]
c      kph--phase flag:  1 = liquid
c                        2 = vapor
c                   N.B.:  0 = stable phase--NOT ALLOWED (use
TPFLSH)
c   kguess--input flag:  1 = first guess for rho provided
c                        0 = no first guess provided
c        rho--first  guess  for  molar  density  [mol/L],  only  if
kguess = 1
c
c  outputs:
c      rho--molar density [mol/L]
c     ierr--error flag:  0 = successful
c                      200 = CRITP did not converge
c                      201 = illegal input (kph <= 0)
```

```
c                        202 = liquid-phase iteration did not
converge
c                         203 = vapor-phase iteration did not
converge
c     herr--error string (character*255 variable if ierr<>0)
```

C.5.3 Two-phase flash subroutines

These routines accept only two-phase (liquid + vapor) states as inputs. They will be faster than the corresponding general routines, but will fail if called with an incorrect phase specification. The phase-specific subroutines also do not check limits, so may fail if called outside the range of the equation of state. The following two-phase routines are available.

```
      subroutine TPFL2 (t,p,z,Dl,Dv,x,y,q,ierr,herr)
      subroutine DHFL2 (D,h,z,t,p,Dl,Dv,x,y,q,ierr,herr)
      subroutine DSFL2 (D,s,z,t,p,Dl,Dv,x,y,q,ierr,herr)
      subroutine DEFL2 (D,e,z,t,p,Dl,Dv,x,y,q,ierr,herr)

c  inputs--two of the following as indicated by the first two
letters of c          the subroutine name:
c        t--temperature [K]
c        p--pressure [kPa]
c        D--bulk molar density [mol/L]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]
c
c  additional inputs--required for all routines
c        z--overall (bulk) composition [array of mol frac]
c     Dmin--lower bound on density [mol/L]
c     Dmax--upper bound on density [mol/L]
c
c  outputs:
c        t--temperature [K] (not present for TPFL2)
c        p--pressure [kPa] (not present for TPFL2)
c       Dl--molar density [mol/L] of the liquid phase
c       Dv--molar density [mol/L] of the vapor phase
c        x--composition of liquid phase [array of mol frac]
c        y--composition of vapor phase [array of mol frac]
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
```

In the following two-phase flash routines, there is the option to pass the dew and bubble point conditions as inputs; if these data are known (from a previous call to SATT or SATP, for example), these two-phase routines will be significantly faster than the corresponding general routines described in Section C.5.1. Otherwise, the general routines will be more reliable.

```
      subroutine                                         TDFL2
(t,D,z,ksat,pbub,pdew,Dlbub,Dvdew,ybub,xdew,
     &                  p,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         TEFL2
(t,e,z,ksat,pbub,pdew,Dlbub,Dvdew,ybub,xdew,
     &                  p,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         THFL2
(t,h,z,ksat,pbub,pdew,Dlbub,Dvdew,ybub,xdew,
     &                  p,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         TSFL2
(t,s,z,ksat,pbub,pdew,Dlbub,Dvdew,ybub,xdew,
     &                  p,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         PDFL2
(p,d,z,ksat,tbub,tdew,Dlbub,Dvdew,ybub,xdew,
     &                  t,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         PEFL2
(p,e,z,ksat,tbub,tdew,Dlbub,Dvdew,ybub,xdew,
    &                  t,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         PHFL2
(p,h,z,ksat,tbub,tdew,Dlbub,Dvdew,ybub,xdew,
     &                  t,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         PSFL2
(p,s,z,ksat,tbub,tdew,Dlbub,Dvdew,ybub,xdew,
    &                  t,Dl,Dv,x,y,q,ierr,herr)
      subroutine                                         TQFL2
(t,q,z,kq,ksat,pbub,pdew,Dlbub,Dvdew,ybub,xdew,
     &                  p,Dl,Dv,x,y,ierr,herr)
      subroutine                                         PQFL2
(p,q,z,kq,ksat,tbub,tdew,Dlbub,Dvdew,ybub,xdew,
     &                  t,Dl,Dv,x,y,ierr,herr)

c  inputs--two of the following as indicated by the first two
letters of c          the subroutine name:
c        t--temperature [K]
c        p--pressure [kPa]
c        D--overall (bulk) molar density [mol/L]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [[J/mol-K]
c
c  additional inputs
c        z--overall (bulk) composition [array of mol frac]
c     ksat--flag for bubble and dew point limits
c            0 = dew and bubble point limits computed within
routine
```

```
c           1 = must provide values for following:
c  additional additional input--only for TQFL2 and PQFL2
c       kq--flag specifying units for input quality
c            kq = 1 quality on MOLAR basis [moles vapor/total
moles]
c             kq = 2 quality on MASS basis [mass vapor/total
mass]
c
c  additional inputs if ksat = 1
c     tbub--bubble point temperature [K] at (p,x=z)
c     tdew--dew point temperature [K] at (p,y=z)
c    --or--
c     pbub--bubble point pressure [kPa] at (t,x=z)
c     pdew--dew point pressure [kPa] at (t,y=z)
```

```
c    --and—
c    Dlbub--liquid density [mol/L] at bubble point
c    Dvdew--vapor density [mol/L] at dew point
c      ybub--vapor composition [array of mol frac] at bubble
point
c       xdew--liquid composition [array of mol frac] at dew
point
c
c  outputs--one of the following, depending on the inputs:
c        t--temperature [K]
c        p--pressure [kPa]
c
c  additional outputs--common to all routines
c       Dl--molar density [mol/L] of the liquid phase
c       Dv--molar density [mol/L] of the vapor phase
c        x--composition of liquid phase [array of mol frac]
c        y--composition of vapor phase [array of mol frac]
c        q--vapor quality on a MOLAR basis [moles vapor/total
moles]
c           (not present for TQFL2 and PQFL2)
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
            subroutine                                   DQFL2
(d,q,z,kq,t,p,Dl,Dv,x,y,ierr,herr)
c
c    flash calculation given bulk density, quality, and
composition
c
c  This routine accepts only two-phase states as input.
c
c  inputs:
c        d--overall (bulk) molar density [mol/L]
c        h--overall (bulk) molar enthalpy [J/mol]
c        z--overall (bulk) composition [array of mol frac]
c       kq--flag specifying units for input quality
c            kq = 1 quality on MOLAR basis [moles vapor/total
moles]
c             kq = 2 quality on MASS basis [mass vapor/total
mass]
c
c  outputs:
c        t--temperature [K]
c        p--pressure [kPa]
c       Dl--molar density [mol/L] of the liquid phase
c       Dv--molar density [mol/L] of the vapor phase
c        x--composition of liquid phase [array of mol frac]
c        y--composition of vapor phase [array of mol frac]
c     ierr--error flag:  0 = successful
c     herr--error string (character*255 variable if ierr<>0)
```

C.6 Thermodynamic Property Subroutines as f(T,ρ,x)

The following routines provide thermodynamic properties as a function of temperature, density, and composition. Typically, one or more of these will be called after finding the temperature and/or density1 with a call to one of the saturation or flash routines. Note that these routines assume that valid inputs are supplied--no range checking is performed.

```
      subroutine CRITP (x,tcrit,pcrit,Dcrit,ierr,herr)
c
c  critical parameters as a function of composition
c
c  input:
c        x--composition [array of mol frac]
c  outputs:
c    tcrit--critical temperature [K]
c    pcrit--critical pressure [kPa]
c    Dcrit--critical density [mol/L]
c     ierr--error flag:  0 = successful
c                        1 = did not converge
c     herr--error string (character*255 variable if ierr<>0)



      subroutine THERM (t,rho,x,p,e,h,s,cv,cp,w,hjt)
c
c  compute thermal quantities as a function of temperature,
density,
c   and compositions using core functions (Helmholtz free
energy, ideal
c  gas heat capacity and various derivatives and integrals)
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  outputs:
c        p--pressure [kPa]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [J/mol-K]
c       Cv--isochoric heat capacity [J/mol-K]
c       Cp--isobaric heat capacity [J/mol-K]
c        w--speed of sound [m/s]
c      hjt--isenthalpic Joule-Thompson coefficient [K/kPa]
      subroutine THERM2 (t,rho,x,p,e,h,s,cv,cp,w,Z,hjt,A,G,
```

```
     &
xkappa,beta,dPdD,d2PdD2,dPdT,dDdT,dDdP,
     &                   spare1,spare2,spare3,spare4)
c
c  compute thermal quantities as a function of temperature,
density,
c  and compositions using core functions (Helmholtz free
energy, ideal
c  gas heat capacity and various derivatives and integrals)
c
c  this routine is similar to THERM, except that additional
properties
c  are calculated
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  outputs:
c        p--pressure [kPa]
c        e--internal energy [J/mol]
c        h--enthalpy [J/mol]
c        s--entropy [J/mol-K]
c       Cv--isochoric heat capacity [J/mol-K]
c       Cp--isobaric heat capacity [J/mol-K]
c        w--speed of sound [m/s]
c        Z--compressibility factor (= PV/RT) [dimensionless]
c      hjt--isenthalpic Joule-Thompson coefficient [K/kPa]
c        A--Helmholtz energy [J/mol]
c        G--Gibbs free energy [J/mol]
c   xkappa--isothermal compressibility [1/kPa]
c           (= -1/V dV/dP = 1/rho dD/dP) [1/kPa]
c      beta--volume expansivity (= 1/V dV/dT = -1/rho dD/dT)
[1/K]
c     dPdD--derivative dP/drho [kPa-L/mol]
c   d2PdD2--derivative d^2P/drho^2 [kPa-L^2/mol^2]
c     dPdT--derivative dP/dT [kPa/K]
c     dDdT--derivative drho/dT [mol/L-K]
c     dDdP--derivative drho/dP [mol/L-kPa]
c   sparei--4 space holders for possible future properties
      subroutine ENTRO (t,rho,x,s)
c
c  compute entropy as a function of temperature, density and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c        s--entropy [J/mol-K]
```

```
      subroutine ENTHAL (t,rho,x,h)
c
c  compute enthalpy as a function of temperature, density,
and
c  composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c        h--enthalpy [J/mol]



      subroutine CVCP (t,rho,x,cv,cp)
c
c  compute isochoric (constant volume) and isochoric
(constant pressure)
c  heat capacity as functions of temperature, density, and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  outputs:
c       cv--isochoric heat capacity [J/mol-K]
c       cp--isobaric heat capacity [J/mol-K]
      subroutine GIBBS (t,rho,x,Ar,Gr)
c
c  compute residual Helmholtz and Gibbs free energy as a
function of
c  temperature, density, and composition
c
c  N.B.  The quantity calculated is
c
c            G(T,rho) - G0(T,P*) = G(T,rho) - G0(T,rho) +
RTln(RTrho/P*)
c
c            where G0 is the ideal gas state and P* is a
reference pressure
c         which is equal to the current pressure of interest.
Since Gr
c          is used only as a difference in phase equilibria
calculations
c         where the temperature and pressure of the phases are
equal, the
c          (RT/P*) part of the log term will cancel and is
omitted.
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
```

```
c        x--composition [array of mol frac]
c  outputs:
c       Ar--residual Helmholtz free energy [J/mol]
c       Gr--residual Gibbs free energy [J/mol]
```

```
      subroutine AG (t,rho,x,a,g)
c
c   compute  Helmholtz  and  Gibbs  energies  as  a  function  of
temperature,
c  density, and composition.
c
c  N.B.  These are not residual values (those are calculated
by GIBBS).
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  outputs:
c        a--Helmholtz energy [J/mol]
c        g--Gibbs free energy [J/mol]
      subroutine PRESS (t,rho,x,p)
c
c  compute pressure as a function of temperature,
c  density, and composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c        p--pressure [kPa]
```

```
      subroutine DPDD (t,rho,x,dpdrho)
c
c  compute partial derivative of pressure w.r.t. density at
constant
c   temperature  as  a  function  of  temperature,  density,  and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c   dpdrho--dP/drho [kPa-L/mol]
```

```
      subroutine DPDD2 (t,rho,x,dp2dD2)
```

```
c
c   compute second partial derivative of pressure w.r.t.
density at const
c   temperature as a function of temperature, density, and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c   d2pdD2--d^2P/drho^2 [kPa-L^2/mol^2]



      subroutine DPDT (t,rho,x,dpt)
c
c  compute partial derivative of pressure w.r.t. temperature
at constant
c   density as a function of temperature, density, and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c      dpt--dP/dT [kPa/K]


      subroutine DDDP (t,rho,x,drhodp)
c
c  compute partial derivative of density w.r.t. pressure at
constant
c   temperature as a function of temperature, density, and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c   drhodp--drho/dP [mol/L-kPa]



      subroutine DDDT (t,rho,x,drhodt)
c
c  compute partial derivative of density w.r.t. temperature
at constant
c   pressure as a function of temperature, density, and
composition
```

```
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c   drhodt--drho/dT [mol/L-K]
c
c   d(rho)/d(T) = -d(rho)/dP x dP/dT = -dP/dT / (dP/d(rho))



      subroutine DHDT (t,rho,x,dht)
c
c  compute partial derivative of enthalpy w.r.t. temperature
at constant
c   density as a function of temperature, density, and
composition
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c      dht--dH/dT [J/mol-K]


      subroutine VIRB (t,x,b)
c
c  compute second virial coefficient as a function of T & x
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c  outputs:
c        b--second virial coefficient [L/mol]


      subroutine DBDT (t,x,dbt)
c
c   compute the 2nd deriviate of B (B is the second virial
coefficient) with
c  respect to T as a function of temperature and composition.
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c  outputs:
c      dbt--2nd deriviate of B with respect to T [L/mol-K]


      subroutine VIRC (t,x,c)
c
```

```
c   compute the third virial coefficient as a function of T &
x
```

```
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c  outputs:
c        c--thrid virial coefficient [(L/mol)^2]
      subroutine VIRD (t,x,d)
c
c   compute the fourth virial coefficient as a function of
temperature
c  and composition.
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c  outputs:
c        d--fourth virial coefficient [(L/mol)^3]



      subroutine FGCTY (t,rho,x,f)
c
c   compute fugacity for each of the nc components of a
mixture by
c   numerical differentiation (using central differences) of
the
c  dimensionless residual Helmholtz energy
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c  output:
c        f--array (1..nc) of fugacities [kPa]



      subroutine EXCESS (t,p,x,vE,eE,hE,sE)
c
c   compute excess properties as a function of temperature,
pressure,
c  and composition.
c
c  inputs:
c        t--temperature [K]
c        p--pressure [kPa]
c        x--composition [array of mol frac]
c  outputs:
c        vE--excess volume [L/mol]
c        eE--excess energy [J/mol]
c        hE--excess enthalpy [J/mol]
c        sE--excess entropy [J/mol-K]
```

C.7 Transport Property Subroutine

```
      subroutine TRNPRP (t,rho,x,eta,tcx,ierr,herr)
c
c  compute the transport properties of thermal conductivity
and
c   viscosity as functions of temperature, density, and
composition
c
c  inputs:
c        t--temperature (K)
c      rho--molar density (mol/L)
c        x--composition array (mol frac)
c  outputs:
c      eta--viscosity (uPa.s)
c      tcx--thermal conductivity (W/m.K)
c     ierr--error flag:  0 = successful
c                      -31 = temperature out of range for
conductivity
c                         -32 = density out of range for
conductivity
c                         -33 = T and D out of range for
conductivity
c                      -41 = temperature out of range for
viscosity
c                         -42 = density out of range for
viscosity
c                         -43 = T and D out of range for
viscosity
c                   -51 = T out of range for both visc and
t.c.
c                   -52 = D out of range for both visc and
t.c.
c                   -53 = T and/or D out of range for visc
and t.c.
c                         39 = model not found for thermal
conductivity
c                       49 = model not found for viscosity
c                       50 = ammonia/water mix (no properties
calculated)
c                        51 = exactly at t_crit, rho_crit for
a pure
c                           fluid; tcx is infinite
c                 -58,-59 = ECS model did not converge
c     herr--error string (character*255 variable if ierr<>0)
```

C.8 Miscellaneous Properties

The following routines return the dielectric constant, melting line, and sublimation line. These properties are not available for all fluids in REFPROP.

```
      subroutine DIELEC (t,rho,x,de)
c
c    compute the dielectric constant as a function of
temperature, density,
c  and composition.
```

```
c
c  inputs:
c        t--temperature [K]
c      rho--molar density [mol/L]
c        x--composition [array of mol frac]
c   output:
c       de--dielectric constant


      subroutine MELTT (t,x,p,ierr,herr)
c
c   compute the melting line pressure as a function of
temperature
c  and composition.
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c   output:
c        p--melting line pressure [kPa]
c        ierr--error flag:  0 = successful
c             herr--error string (character*255 variable if
ierr<>0)


      subroutine MELTP (p,x,t,ierr,herr)
c
c   compute the melting line temperature as a function of
pressure
c  and composition.
c
c  inputs:
c        p--melting line pressure [kPa]
c        x--composition [array of mol frac]
c   output:
c        t--temperature [K]
c        ierr--error flag:  0 = successful
c             herr--error string (character*255 variable if
ierr<>0)
      subroutine SUBLT (t,x,p,ierr,herr)
c
c   compute the sublimation line pressure as a function of
temperature
c  and composition.
c
c  inputs:
c        t--temperature [K]
c        x--composition [array of mol frac]
c   output:
c        p--sublimation line pressure [kPa]
c        ierr--error flag:  0 = successful
c             herr--error string (character*255 variable if
ierr<>0)
```

```
      subroutine SUBLP (p,x,t,ierr,herr)
c
c  compute the sublimation line temperature as a function of
pressure
c  and composition.
c
c  inputs:
c        p--sublimation line pressure [kPa]
c        x--composition [array of mol frac]
c   output:
c        t--temperature [K]
c        ierr--error flag:  0 = successful
c             herr--error  string  (character*255  variable  if
ierr<>0)
```

C.9 Utility Subroutines

The following "utility" routines provide fluid constants, such as the molecular weight, and provide conversions between mass and molar quantities.

```
      subroutine                                         INFO
(icomp,wm,ttp,tnbp,tc,pc,Dc,Zc,acf,dip,Rgas)
c
c  provides fluid constants for specified component
c
c  input:
c    icomp--component number in mixture; 1 for pure fluid
c  outputs:
c       wm--molecular weight [g/mol]
c      ttp--triple point temperature [K]
c     tnbp--normal boiling point temperature [K]
c       tc--critical temperature [K]
c       pc--critical pressure [kPa]
c       Dc--critical density [mol/L]
c                  Zc--compressibility   at   critical   point
[pc/(Rgas*Tc*Dc)]
c      acf--accentric factor [-]
c      dip--dipole moment [debye]
c     Rgas--gas constant [J/mol-K]



      subroutine NAME (icomp,hname,hn80,hcas)
c
c  provides name information for specified component
```

```
c
c  input:
c    icomp--component number in mixture; 1 for pure fluid
c  outputs:
c    hname--component name [character*12]
c     hn80--component name--long form [character*80]
c           hcas--CAS  (Chemical  Abstracts  Service)  number
[character*12]


      function WMOL (x)
c
c  molecular weight for a mixture of specified composition
c
c  input:
c        x--composition array [array of mol frac]
c
c  output (as function value):
c     WMOL--molar mass [g/mol], a.k.a. "molecular weight"



      subroutine XMASS (xmol,xkg,wmix)
c
c   converts  composition  on  a  mole  fraction  basis  to  mass
fraction
c
c  input:
c     xmol--composition array [array of mol frac]
c  outputs:
c      xkg--composition array [array of mass frac]
c         wmix--molar  mass  of  the  mixture  [g/mol],  a.k.a.
"molecular weight"



      subroutine XMOLE (xkg,xmol,wmix)
c
c   converts  composition  on  a  mass  fraction  basis  to  mole
fraction
c
c  input:
c      xkg--composition array [array of mass frac]
c  outputs:
c     xmol--composition array [array of mol frac]
c         wmix--molar  mass  of  the  mixture  [g/mol],  a.k.a.
"molecular weight"


      subroutine                                        QMOLE
(qkg,xlkg,xvkg,qmol,xl,xv,wliq,wvap,ierr,herr)
c
c   converts  quality  and  composition  on  a  mass  basis  to  a
molar basis
```

```
c
c  inputs:
c      qkg--quality on mass basis [mass of vapor/total mass]
c           qkg = 0 indicates saturated liquid
c           qkg = 1 indicates saturated vapor
c           0 < qkg < 1 indicates a two-phase state
c              qkg < 0 or qkg > 1 are not allowed and will
result in warning
c      xlkg--mass composition of liquid phase [array of mass
frac]
c      xvkg--mass composition of vapor phase [array of mass
frac]
c  outputs:
c     qmol--quality on mass basis [mass of vapor/total mass]
c        xl--molar composition of liquid phase [array of mol
frac]
c        xv--molar composition of vapor phase [array of mol
frac]
c     wliq--molecular weight of liquid phase [g/mol]
c     wvap--molecular weight of vapor phase [g/mol]
c     ierr--error flag:  0 = all inputs within limits
c           -19:  input q < 0 or > 1
c     herr--error string (character*255 variable if ierr<>0)



      subroutine                                        QMASS
(qmol,xl,xv,qkg,xlkg,xvkg,wliq,wvap,ierr,herr)
c
c  converts quality and composition on a mole basis to a mass
basis
c
c  inputs:
c     qmol--molar quality [moles vapor/total moles]
c           qmol = 0 indicates saturated liquid
c           qmol = 1 indicates saturated vapor
c           0 < qmol < 1 indicates a two-phase state
c             qmol < 0 or qmol > 1 are not allowed and will
result in warning
c       xl--composition of liquid phase [array of mol frac]
c       xv--composition of vapor phase [array of mol frac]
c  outputs:
c      qkg--quality on mass basis [mass of vapor/total mass]
c      xlkg--mass composition of liquid phase [array of mass
frac]
c      xvkg--mass composition of vapor phase [array of mass
frac]
c     wliq--molecular weight of liquid phase [g/mol]
c     wvap--molecular weight of vapor phase [g/mol]
c     ierr--error flag:  0 = all inputs within limits
c           -19:  input q < 0 or > 1
c     herr--error string (character*255 variable if ierr<>0)
      subroutine                                       LIMITX
(htyp,t,D,p,x,tmin,tmax,Dmax,pmax,ierr,herr)
```

```
c
c   returns limits of a property model as a function of
composition
c  and/or checks input t, D, p against those limits
c
c   Pure fluid limits are read in from the .fld files; for
mixtures, a
c   simple mole fraction weighting in reduced variables is
used.
c
c   Attempting calculations below the mininum temperature
and/or above
c  the maximum density will result in an error.  These will
often
c  correspond to a physically unreasonable state; also many
equations of
c  state do not extrapolate reliably to lower T's and higher
D's.
c
c   A warning is issued if the temperature is above the
maximum but below
c  1.5 times the maximum; similarly pressures up to twice the
maximum
c  result in only a warning. Most equations of state may be
c  extrapolated to higher T's and P's.  Temperatures and/or
pressures
c  outside these extended limits will result in an error.
c
c   When temperature is unknown, set t to -1 to avoid
performing
c  the melting line check
c
c  inputs:
c      htyp--flag indicating which models are to be checked
[character*3]
c               'EOS':  equation of state for thermodynamic
properties
c           'ETA':  viscosity
c           'TCX':  thermal conductivity
c           'STN':  surface tension
c        t--temperature [K]
c        D--molar density [mol/L]
c        p--pressure [kPa]
c        x--composition array [mol frac]
c      N.B.--all inputs must be specified, if one or more are
not
c              available, (or not applicable as in case of
surface tension)
c           use reasonable values, such as:
c           t = tnbp
c           D = 0
c           p = 0
c  outputs:
```

```
c      tmin--minimum temperature for model specified by htyp
[K]
c     tmax--maximum temperature [K]
c     Dmax--maximum density [mol/L]
c     pmax--maximum pressure [kPa]
c     ierr--error flag:  0 = all inputs within limits
c                            <>0 = one or more inputs outside
limits:
c                        -1 = 1.5*tmax > t > tmax
c                         1 = t < tmin or t > 1.5*tmax
c                         2 = D > Dmax or D < 0
```

```
c                       -4 = 2*pmax > p > pmax
c                        4 = p < 0 or p > 2*pmax
c                        8 = component composition < 0 or > 1
c                             and/or composition sum < 0 or >
1
c                       16 = p>pmelt
c                      -16 = t<ttrp (important for water)
c              if multiple inputs are outside limits, ierr =
abs[sum(ierr)]
c               with the sign determined by the most severe
excursion
c              (ierr > 0 indicate an error--calculations not
possible,
c                ierr < 0 indicate a warning--results may be
questionable)
c     herr--error string (character*255 variable if ierr<>0)



      subroutine                                       LIMITK
(htyp,icomp,t,D,p,tmin,tmax,Dmax,pmax,ierr,herr)
c
c  returns limits of a property model (read in from the .fld
files) for
c  a mixture component and/or checks input t, D, p against
those limits
c
c  This routine functions in the same manner as LIMITX except
that the
c  composition x is replaced by the component number icomp.
c
c   See the description of LIMITX for input and output
information.



      subroutine ERRMSG (ierr,herr)
c
c  write error messages to default output; this subroutine
should be
c  called immediately after any call to a subroutine which
potentially
c  can error out
c
c  inputs:
c      ierr--error flag:  0 = successful (no message will be
written)
c                       <0 = warning
c                       >0 = error
c     herr--error string (character*255 variable)
c
c  outputs:
c     none--error string written to default output
c
```

```
c      N.B.  the statement which writes output to the screen
is
c             commented out to avoid problems with the DLL;
this must be
c           uncommented if you wish to see error messages on
the screen;
c               alternately, open a file from within your
application and
c                replace the "write (*,1000)" with "write
(unit=i,1000)" to
c            write the messages to that file (where i is a
logical unit)
```

C.10 Differences With Version 6 FORTRAN Routines

Compared to version 6, version 7 of REFPROP includes many additional routines providing additional properties and calculation options, including:

- the maximum number of components in a mixture has been increased to 20,
- the addition of dielectric constant, melting line, and sublimation line data for some fluids,
- saturation states may be specified by the density, enthalpy, or entropy in addition to the existing temperature and pressure routines,
- many additional flash combinations with virtually all combinations of temperature, pressure, density, internal energy, enthalpy, entropy, or quality are supported, and
- the flash routines with vapor quality as an input now accept quality on either a mass or molar basis.

All version 6 subroutines are retained with the same inputs and outputs. One change to the existing routines is that the file specification variables “hfiles” and “hfmix” used in SETUP, SETKTV, and GETKTV have been changed from character*80 to character*255. This was needed to accomodate the very long path names used on some systems. These routines can detect, in most cases, if the input variable is declared as character*80, so existing programs should work without modification.

A number of common blocks holding fluid constants have been changed to accomodate new models. Users have been cautioned against refering to common blocks. The routines INFO, NAME, WMOL, etc. should be used when fluid constants are required.

Appendix D

USING THE REFPROP DLL

Two dynamic link libraries (DLLs) are provided with REFPROP. The file REFPROP.DLL is used by the graphical interface and can be accessed by Excel spreadsheets and Visual Basic programs. The file refp32.DLL implements the calling conventions used in version 6 of REFPROP. It is provided for compatibility with older codes.

D.1 Excel Spreadsheets

A sample Excel spreadsheet is available that demonstrates the use of Excel with REFPROP. The file is named REFPROP.xls and is located in the directory where the REFPROP application was installed.

Properties are calculated by calling various functions. The following functions are available:

Temperature
Pressure
Density
LiquidDensity
VaporDensity
Volume
Energy
Enthalpy
Entropy
IsochoricHeatCapacity (or: Cv)
IsobaricHeatCapacity (or: Cp)
SpeedOfSound (or: Sound)
Quality
Viscosity
ThermalConductivity
SurfaceTension

For example, the following line would be placed in a cell to calculate the density of argon at 300 K and 10 MPa:

```
=Density("argon","TP",,300,10)
```

The first input in the call to the function is the pure fluid name or mixture string. The file name located in the fluids directory where REFPROP was installed should be used as the fluid name (without the .fld extension).

For mixtures, the fluid names and compositions (in mole fractions) of the constituents in the mixture are placed in a single cell as in the following example for dry air:

```
nitrogen,0.7812,argon,0.0092,oxygen,0.2096
```

A more convenient way is to use the CONCAT phrase to join multiple cells:

```
=CONCATENATE(A1,",",B1,",",A2,",",B2,",",A3,",",B3)
```

where the fluid names are stored in A1, A2, and A3, and the mole fractions are stored in B1, B2, and B3.

The second input to the function is the combination of input properties being sent to the function. Thus, for a given pressure and temperature, the second input would be "PT" (or "TP", depending on the order that the properties are sent.) Other valid inputs include the density (D), volume (V), energy (E), enthalpy (H), entropy (S), and quality (Q). Valid combinations include: TP, TD, TH, TS, TE, TQ, PD, PS, PE, PQ, DH, DS, and DE. For saturation states, the second input is just T given a saturated temperature, P for a given saturated pressure, or D for a saturated density. The vapor properties are returned for density, enthalpy, etc. To define liquid or vapor inputs, use TLIQ, TVAP, PLIQ, or PVAP instead of just T or P.

The third input to the property functions defines the units. This input can be one of the following: SI, E, cgs, mks, M. The default (if left blank) is SI. The units that correspond to these inputs are for temperature, pressure, density, enthalpy, entropy and heat capacity, sound speed, viscosity, and thermal conductivity:

SI: K, MPa, mol/L, J/mol, J/mol-K, m/s, uPa-s, mW/m-K
mks: K, kPa, kg/m^3, kJ/kg, kJ/kg-K, m/s, uPa-s, W/m-K
cgs: K. MPa, g/cm^3, J/g, J/g-K, cm/s, uPa-s, mW/m-K
E: F, psia, lb/ft^3, Btu/lb, Btu/lb-R, ft/s, lb/ft-s, Btu/h-ft-F
M: K, psia, g/cm^3, J/g, J/g-K, m/s, uPa-s, mW/m-K

For example, the following line would be placed in a cell to calculate the density of argon at 100 F and 250 psia:

```
=Density("argon","TP",E,100,250)
```

The independent variables in the equations of state used in REFPROP are temperature and density. If more than one property is needed, it is best to first determine these quantities from the given set of initial inputs, and then determine the other properties. This will greatly enhance the calculation speed in processes using numerous calculations. This is particularly important when calculating properties for pure fluids that are within the two phase. For example, to calculate the energy, enthalpy, and entropy given the pressure and quality of a two phase system, place the fluid name in cell A1, the pressure in B1, and the quality in C1. Put the following in cells A2 through E2

```
=Temperature($A$1,"PQ",,$B$1,$C$1)
=Density($A$1,"PQ",,$B$1,$C$1)
=Energy($A$1,"TD",,$A$2,$B$2)
=Enthalpy($A$1,"TD",,$A$2,$B$2)
=Entropy($A$1,"TD",,$A$2,$B$2)
```

The functions LiquidDensity and VaporDensity will return the saturated liquid and vapor densities of a two phase state. These densities, along with the temperature, can then be used to calculate all other thermodynamic and transport properties at the saturation boundaries using the functions outlined above.

The file REFPROP.DLL is used by the Excel spreadsheet.

D.2 Visual Basic Programs

A sample Visual Basic code is provided that demonstrates the use of VB with REFPROP. The file is called Sample.Bas and is located in the directory where the REFPROP program was installed. It uses the dynamic link library REFPROP.DLL.

VB subroutines analogous to all of the FORTRAN subroutines described in Sections C.3 through C.9 are available. The subroutine names have “dll” appended to the FORTRAN names (for example, SETUPdll is the VB analog to the FORTRAN subroutine SETUP). The inputs and outputs are the same as the FORTRAN routines, except that additional arguments specifying the length of any string variables are required.

The file Sample.bas consists of subroutine and variable declarations in the first part of the file. These declarations would be necessary for any program. The latter part of the file provides examples of calling the various subroutines. No output is displayed when the program is run, it is intended only to show how the calling routines work. Comments are given throughout the code describing the various calls and procedures. Additional details on the subroutines and functions are given in the FORTRAN code included with REFPROP.

D.3 Sample C++ Code

A C++ example program, called RefDemo.Cpp and located in the Cpp.zip file, is available to illustrate linking C++ code with the routines used in REFPROP. The file is located in the directory where the REFPROP program was installed.

The example was written by Dave Richardson at the University of Maryland and shows how the calling routines work. The example code links the Refdemo program to the REFPROP.dll file statically. If the user wishes to link in a similar manner, they must create the REFPROP.lib file which will work with their compiler. An alternative to static linking would be to link dynamically at run time, but this is not demonstrated in the example.

D.4 Sample MatLab Code

A sample MatLab file, called property.f90 and located in the MatLab.zip file, is available to illustrate linking MatLab with the routines used in REFPROP. The file is located in the directory where the REFPROP program was installed.

The example was written by Lennart Vamling at Chalmers University of Technology in Sweden and shows how the calling routines work. To test the sample program:

1. The REFPROP fluids directory should be located in C:\Program Files\REFPROP\fluids
2. The MatLab path should include the directory where the (unzipped) files property.dll and property.m reside.

Otherwise, to adopt to another fluids directory location, one line in the property.f90 file has to be changed to reflect the directory used, and then it must be recompiled using the MatLab “mex” command. MatLab must then be configured to work with a suitable FORTRAN compiler. The REFPROP subroutines must also be referenced in the mex command.

Some users of the MatLab interface have experienced that the first call gave strange answers, but an identical second call gave the correct result.

Appendix E

WARNING AND ERROR MESSAGES

The FORTRAN routines return warning and error codes and messages when the input conditions are out of range or the calculations fail. The error codes are integers returned in the subroutine argument *ierr*. When a calculation is successful, the value of *ierr* is 0. Negative values of *ierr* signify a warning—that is, a condition where calculations were completed, but the results may be suspect. The most common warning would be for a temperature or pressure slightly above the limits of the property model.

Errors imply conditions for which the calculations failed (such as an iteration not converging) or for which calculations are not possible (such as a negative pressure or a mixture composition not summing to one). Many property models give nonsensical results when extrapolated to lower temperatures and/or higher densities, thus, errors are also issued when the temperature is below the limit of the model or the density is above the limit. The codes for errors are positive numbers.

More detailed messages (including, in some cases, a report of the input condition(s) which resulted in the warning or error) are available via the output variable herr, which may be printed or displayed using the subroutine ERRMSG. In the interface, errors are displayed in an Alert box. If the calculation of a table results in a warning, a message is displayed at the completion of the calculations, and the individual messages can be displayed by clicking the mouse on the number of the affected row.

A listing of warning/error codes is provided below. Codes related to temperature, pressure, and composition limits are common to many routines. Some codes for the flash routines are listed twice because a "general" flash routine may call a subsidiary routine for a specified phase (for example, TPFLSH may call TPRHO or PFL2); if the subsidiary routine generates an error, it is passed back to the general routine.

Limits-related warning messages for thermodynamic properties (apply to all saturation and flash routines):

-1 = Tin > Tmax
-4 = Pin > Pmax
-5 = Tin > Tmax and Pin > Pmax

Limits-related error messages for thermodynamic properties (apply to all saturation and flash routines):

1 = Tin < Tmin
2 = Din > Dmax or Din < 0
3 = T and D out of range
4 = Pin < 0
5 = T and P out of range
6 = D and P out of range
7 = T and D and P out of range
8 = x out of range (component and/or sum < 0 or > 1)
9 = x and T out of range
10 = x and D out of range
11 = x and T and D out of range
12 = x out of range and P < 0
13 = x and T and P out of range
14 = x and D and P out of range

Thermal conductivity (TRNPRP)

-31 = temperature out of range
-32 = density out of range
-33 = T and D out of range
-35 = temperature out of range for reference fluid (ECS--conductivity)

-36 = density out of range for reference fluid (ECS--conductivity)
-37 = T and D out of range for reference fluid (ECS--conductivity)
39 = specified model not implemented

Viscosity (TRNPRP)

-41 = temperature out of range
-42 = density out of range
-43 = T and D out of range
-45 = temperature out of range for reference fluid (ECS--viscosity)
-46 = density out of range for reference fluid (ECS--viscosity)
-47 = T and D out of range for reference fluid (ECS--viscosity)
49 = specified model not implemented

Combined warnings for thermal conductivity and viscosity (TRNPRP)

50 = ammonia/water mixture (no properties calculated)
51 = exactly at critical for a pure fluid; tcx is infinite
-51 = temperature out of range
-52 = density out of range
-53 = T and/or D out of range for t.c. and/or visc
-54 = failure of critical point routine (ECS method)
-55 = T out of range for both visc and t.c. (ECS method)
-56 = D out of range for both visc and t.c. (ECS method)
-57 = T and/or D out of range for both visc and t.c. (ECS method)
-58 = iteration to find temperature and/or density reducing ratios f,h did not converge (ECS method)
-59 = iteration to find temperature reducing ratio f did not converge

Initialization routines (SETUP, SETREF, SETMOD, SETKTV, GETKTV) reference state setup errors/warnings:
22 = Tmin > Tref for IIR reference state
23 = Tcrit < Tref for IIR reference state
24 = Tmin > Tref for ASHRAE reference state
25 = Tcrit < Tref for ASHRAE reference state
26 = Tmin > Tnbp for NBP reference state
27 = Tref,Pref for OTH ref state outside EOS limits
-28 = can't apply 'DEF' to mix; will apply to pures
-29 = unknown reference state specified; will use 'DEF'
model setup errors/warnings:
101 = error in opening file
102 = error in file or premature end of file
-103 = unknown model encountered in file
104 = error in setup of model
105 = specified model not found
mixture setup errors/warnings:
111 = error in opening mixture file
112 = mixture file of wrong type
-113 = illegal i,j specification (i=j or i>nc or j>nc)
-114 = critical temperature line will be estimated
-115 = critical volume line will be estimated
-116 = critical temperature and volume will be estimated
-117 = binary pair not found, parameters will be estimated
118 = error in reading mixture file
119 = convergence failure is calculating reference state

Saturation conditions given temperature (SATT)
0 = successful
1 = T < Tmin
8 = x out of range
9 = T and x out of range
120 = CRITP did not converge
121 = T > Tcrit
122 = TPRHO-liquid did not converge (pure fluid)
123 = TPRHO-vapor did not converge (pure fluid)
124 = pure fluid iteration did not converge

The following 3 error codes are advisory--iteration will either converge on later guess or error out (ierr = 128):
-125 = TPRHO did not converge for parent ph (mix)
-126 = TPRHO did not converge for incipient (mix)
-127 = inner (composition) iteration did not converge
128 = mixture iteration did not converge

Saturation conditions given pressure (SATP)
0 = successful
4 = P < 0
8 = x out of range
12 = P and x out of range
140 = CRITP did not converge
141 = P > Pcrit
142 = TPRHO-liquid did not converge (pure fluid)
143 = TPRHO-vapor did not converge (pure fluid)
144 = pure fluid iteration did not converge
The following 4 error codes are advisory--iteration will either converge on later guess or error out (ierr = 148):
-144 = Raoult's law (mix initial guess) has not converged
-145 = TPRHO did not converge for parent phase (mix)
-146 = TPRHO did not converge for incipient phase (mix)
-147 = inner (composition) iteration did not converge
148 = mixture iteration did not converge

Surface tension (SURFT)
0 = successful
1 = T > Tmax
8 = x out of range
9 = T and x out of range
-21 = T < Tmin (surface tension usually extrapolates well)
160 = CRITP did not converge
161 = T > Tcrit
122 = TPRHO-liquid did not converge in SATT
123 = TPRHO-vapor did not converge in SATT
124 = SATT pure fluid iteration did not converge
128 = SATT mixture iteration did not converge

Single-phase temperature-pressure flash (TPRHO)

200 = CRITP did not converge
201 = illegal input (kph <= 0)
202 = liquid-phase iteration did not converge
203 = vapor-phase iteration did not converge
N.B. no limits checking of input variables

General temperature-pressure flash (TPFLSH)

1 = Tin < Tmin
4 = Pin < 0
5 = T and P out of range
8 = x out of range (component and/or sum < 0 or > 1)
9 = x and T out of range
12 = x out of range and P < 0
13 = x and T and P out of range
210 = CRITP did not converge
211 = SATT did not converge at bubble point
212 = SATT did not converge at dew point
213 = TPRHO did not converge for liquid state
214 = TPRHO did not converge for vapor state
215 = TPRHO did not converge for supercritical state
216 = TPRHO did not converge for liq in 2-phase iteration
217 = TPRHO did not converge for vapor in 2-phase iteration
218 = inner loop (liquid frac) for 2-phase iteration did not converge
219 = outer loop (composition) for 2-phase iteration did not converge

Two-phase temperature-pressure flash (TPFL2)

216 = TPRHO did not converge for liquid
217 = TPRHO did not converge for vapor
218 = inner loop (liquid frac) iteration did not converge
219 = outer loop (composition) iteration did not converge

General temperature-density flash (TDFLSH)

1 = Tin < Tmin
2 = Din > Dmax or Din < 0
3 = T and D out of range
8 = x out of range (component and/or sum < 0 or > 1)
9 = x and T out of range
10 = x and D out of range
11 = x and T and D out of range
220 = CRITP did not converge
221 = SATT did not converge at bubble point
222 = SATT did not converge at dew point
223 = SATT did not converge at bubble point from within 2-phase iteration
224 = SATT did not converge at dew point from within 2-phase iteration
225 = TPFL2 within 2-phase iteration did not converge
226 = 2-phase iteration did not converge

Two-phase temperature-density flash (TDFL2)

223 = SATT did not converge at bubble point
224 = SATT did not converge at dew point
225 = TPFL2 from within iteration did not converge
226 = 2-phase iteration did not converge

General pressure-enthalpy flash (PHFLSH)

4 = Pin < 0
8 = x out of range (component and/or sum < 0 or > 1)
12 = x out of range and P < 0
240 = CRITP did not converge
241 = SATP did not converge at bubble point
242 = SATP did not converge at dew point
243 = SATP did not converge at bubble point from within 2-phase iteration
244 = SATP did not converge at dew point from within 2-phase iteration
245 = TPFL2 called from within 2-phase iteration did not converge

246 = 2-phase iteration did not converge
247 = TPRHO did not converge from within single-phase iteration
248 = single-phase iteration did not converge
249 = H out of range

Single-phase pressure-enthalpy flash (PHFL1)
247 = TPRHO did not converge
248 = single-phase iteration did not converge

Two-phase pressure-enthalpy flash (PHFL2)
243 = SATP did not converge at bubble point
244 = SATP did not converge at dew point
245 = TPFL2 called from within iteration did not converge
246 = 2-phase iteration did not converge

General pressure-entropy flash (PSFLSH)
4 = Pin < 0
8 = x out of range (component and/or sum < 0 or > 1)
12 = x out of range and P < 0
260 = CRITP did not converge
261 = SATP did not converge at bubble point
262 = SATP did not converge at dew point
263 = SATP did not converge at bubble point from within 2-phase iteration
264 = SATP did not converge at dew point from within 2-phase iteration
265 = TPFL2 called from within 2-phase iteration did not converge
266 = 2-phase iteration did not converge
267 = TPRHO did not converge from within single-phase iteration
268 = single-phase iteration did not converge
269 = S out of range

Single-phase pressure-entropy flash (PSFL1)
267 = TPRHO did not converge
268 = single-phase iteration did not converge

Two-phase pressure-entropy flash (PSFL2)

263 = SATP did not converge at bubble point
264 = SATP did not converge at dew point
265 = TPFL2 called from within iteration did not converge
266 = 2-phase iteration did not converge

Temperature-quality flash (TQFLSH)
1 = T < Tmin
8 = x out of range
9 = T and x out of range
270 = CRITP did not converge
271 = T > Tcrit
275 = q out of range
278 = TQFLSH did not converge

Pressure-quality flash (PQFLSH)
0 = successful
4 = P < 0
8 = x out of range
9 = P and x out of range
290 = CRITP did not converge
291 = P > Pcrit
295 = q out of range
298 = PQFLSH did not converge

Appendix F

CONTACTS

If you have comments or questions about the database, the Standard Reference Data Program would like to hear from you. Also, if you should have any problems with the diskettes or installation, please let us know by contacting:

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