NIST

NIST Reference Fluid Thermodynamic and Transport Properties— REFPROP

Version 8.0

User's Guide

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ACKNOWLEDGEMENTS

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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, especially natural gas systems.

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 that applies mixing rules 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, an ECS method, or in some cases the friction theory 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 for a specified (T,x) or (P,x) state. Flash calculations describe single- or two-phase states given a wide variety of input combinations $[(P,h,x), (P,T,x), \text{etc}]$.

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 user-specified mixtures or a number of predefined mixtures (air and the commercially available refrigerant blends). A 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 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 4.5.1 and 4.6.)

The user is further cautioned that, by the very nature of a calculational program, 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 User's Guide

Section 2 details the installation procedure. Section 3 presents a brief overview of the structure of the program and its main features. Sections 4 through 11 describe the features of the program in detail. The fluids in the database are tabulated in Appendix A. Use of the FORTRAN property subroutines is described in Appendix B. Use of the property routines with Excel spreadsheets and Visual Basic programs is outlined in Appendix B. Appendix C lists support contacts at NIST.

2. INSTALLATION

2.1 System Requirements

REFPROP is designed to run on any personal computer running the Microsoft® Windows® 98, 2000, XP, or similar operating system. The program requires 20 MB of hard disk space.

2.2 Installation

Place the REFPROP CD-ROM in the CD drive. Click [START], select [RUN] type in: D:\setup, or whichever driver letter is associated with your CD reader. Follow the remainder of the installation instructions.

3. OVERVIEW

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

3.1 Database Structure

REFPROP consists of a graphical user interface (GUI) and FORTRAN 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 B. The DLL can also be utilized by other applications, such as spreadsheets, as described in Appendix B.

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 program. 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 program 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 help system. Clicking the "Continue" button starts the program. 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.
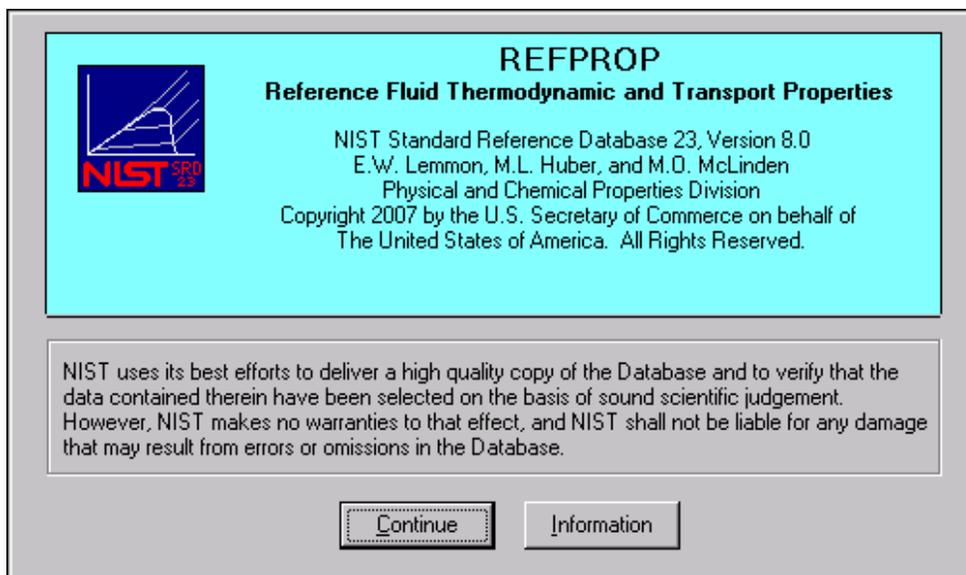
3.3 Overview of the Menus

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 over 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 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.

3.4 Cautions

Users of the REFPROP program should be aware of several potential pitfalls:

If you experience large differences in your expected values of enthalpy or entropy as compared to those calculated by the program, see the information on reference states given in Section 7.2.

The equation parameters for mixtures composed of natural gas fluids come from the 2004 GERG model (see reference in Help file). The default pure fluid equations of state in REFPROP are not the same as those used in the GERG model, rather they are more complex with lower uncertainties. The GERG equations for the pure fluids are shorter, less complex, and faster, but slightly less accurate. To use the GERG model, as published, choose the corresponding option under Options/Preferences. The preference screen also has an option to use the AGA8 model for calculations.

The NIST REFPROP program is designed to provide the most accurate thermophysical properties currently available for pure fluids and their mixtures. The present version is limited to vapor-liquid equilibrium (VLE) only and does not address liquid-liquid equilibrium (LLE), vapor-liquid-liquid equilibrium (VLLE) or other

complex forms of phase equilibrium. The program does not know the location of the freezing line for mixtures. Certain mixtures can potentially enter into these areas without giving warnings to the user.

Some mixtures have components with a wide range of volatilities, as indicated by a critical temperature ratio greater than 2. Certain calculations, especially saturation calculations, may fail without generating warnings. Plotting the calculation results may reveal such cases--looking for discontinuities in density is a good check. Such mixtures, including many with hydrogen, helium, or water, may not have Type I critical behavior, that is they do not have a continuous critical line from one pure component to the other. The estimated critical parameters specified in the Substance/Fluid Information screen for these types of mixtures are represented by a simple linear combination of the pure component values and are not indicative of the true values.

There are cases where an input state point can result in two separate valid states. The most common is temperature-enthalpy inputs. Viewing a T-H diagram will help show how there can be two valid states points for a given input. For example, nitrogen at 140 K and 1000 J/mol can exist at 6.85 MPa and at 60.87 MPa. When this situation occurs, REFPROP returns the state with the higher density. See the Specified State Points text given in Section 5.3 for information on calculating the upper and lower roots.

There are certain properties pertaining only to the saturation line, such as dp/dT. For most cases, displayed properties at saturation states are those for the single phase on the saturation boundary. Thus, derivative properties at saturation as well as saturation properties that are given along constant property paths, such as Cv, Cp, or Csat, pertain to their state in the single phase. Those properties label with a "[sat]" indicate a path along the saturation line.

For pure fluids, when the "Show 2-phase" option in the plot menu is selected, the generated lines for pressure and temperature represent metastable fluid states and the calculated lines between them. These are calculations from the equation of state disregarding any saturation states and generally have no physical significance.

Changing the units in the "Options/Units" menu does not change the units on the tables already created, but only for new tables and plots.

Two equations of state are available for hydrogen to account for the different quantum states of the molecule. Normal hydrogen should be used in applications where it was created and stored at 250 K or above, or when it was cooled to below 250 K and stored without a catalyst for less than a day. The parahydrogen equation should be used where hydrogen was catalyzed or stored for several days at the normal boiling point (NBP) and used at any temperature within 1 day of storage at the NBP. Since the rate of conversion between quantum states is dependent on temperature, pressure, and the storage container, these values are only estimates. For more information, see the Leachman et al. literature reference in the Fluid Information window for hydrogen.

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

The Substance menu defines the fluid or mixture for subsequent property 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 program 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 4.5.1. By clicking the OK button, all subsequent property calculations are carried out on the selected fluid. If you want to retain the previous fluid choice, click the Cancel button.

If a fluid set has been specified (see section 4.4.3), then the "All fluids" button will display all of the fluids available, not just those in the specified set. The pure fluids can be sorted by short name (or nickname), full name, CAS number, chemical formula, synonym, or UN number. This is useful for fluids such as acetone, which is often called propanone, where the name known to the user may not be listed in one of the categories.
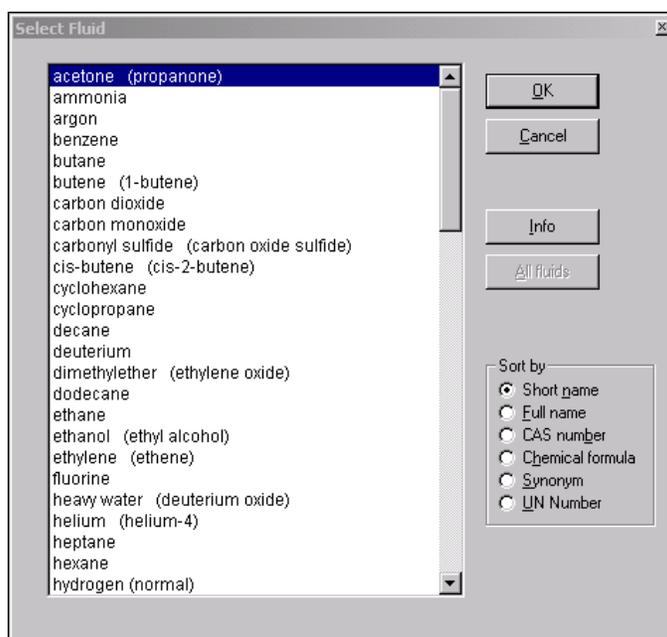
4.2 Selecting a Pseudo Pure Fluid

The Pseudo Pure Fluid dialog lists all of the mixtures with specified compositions that are available as pseudo pure fluids. Select the fluid you want to use by clicking on the fluid name. Click the Info button to display the Fluid Information dialog, which provides critical constants and other property information for the selected fluid.

The properties that are calculated for pseudo pure fluids are based on equations of state that have been developed solely for the specified composition. They are generally based on mixture models that were fit to a wide variety of properties at various compositions. The uncertainties of the pseudo pure fluid equations are

often not as good as the corresponding mixture model; however, the calculational speed will be much higher, especially for saturation properties.
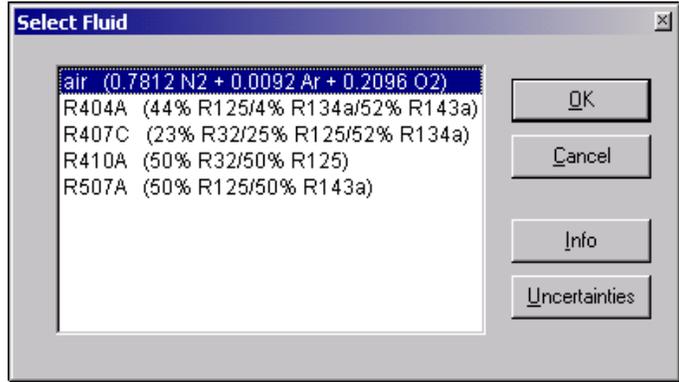
4.3 Selecting a Predefined Mixture

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 4.4. One significant difference between the Pure Fluid and Predefined Mixture dialogs is the effect of the Info button. Clicking the Info button here brings up a Mixture Information screen as described in Section 4.5.3.
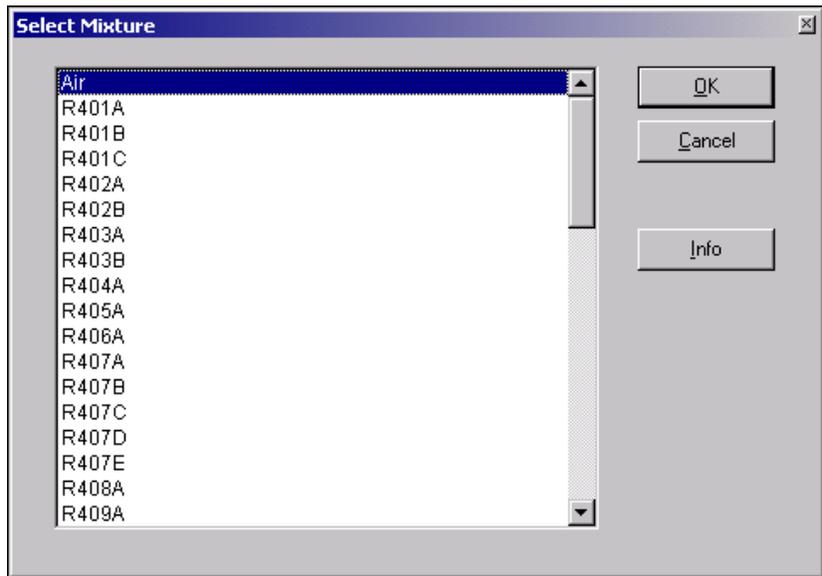
4.4 Defining a New Mixture

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). Note that when a fluid is added to the list on the right, 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.
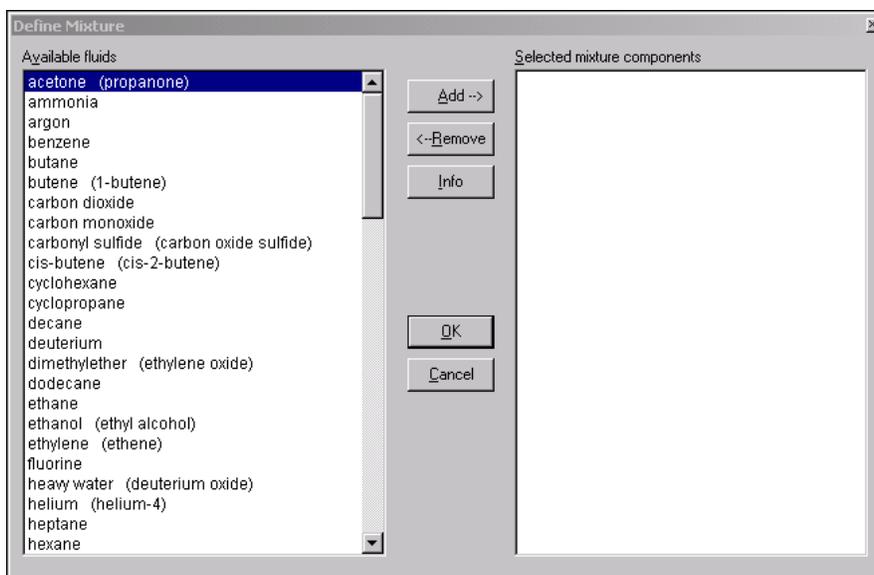
In addition, multiple selections can be made by either holding down the Ctrl key while selecting multiple fluids, or by holding down the Shift key to mark all fluids between the currently marked fluid and the selected one. You can also use the arrow keys to select a fluid, and press Alt-A to add it. 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".

These alternate ways of adding fluids make it easier to find and select a fluid. For example, defining a mixture of R32, R125, R134a, and propane is quickest by typing the following sequence: "r3.r125.r134.pr." If a wrong letter or number is entered, use the backspace button. For instance, if "r124" is entered instead of "r125", press the backspace and then a "5", and the program will jump to R125.

4.4.1 Defining the mixture name and composition

The Specify Mixture 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 4.3).

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.

The mass or mole fractions must be entered for each component and must sum to 1 (or 100 if percentages are used) if the "Normalize compositions to one" checkbox is not selected. If the "Normalize compositions to one" checkbox is selected, the value of each mass or mole fraction is set to the entered value divided by the sum of the values. This option is most convenient if you want to specify the composition of a mixture by specifying the mass of each component.

The Add or Remove Fluid buttons allow you to enter or delete fluids in the list without having to start back at the Define New Mixture dialog. The Add Fluid button will bring up the pure fluid list and the desired

component should be selected. To remove a fluid, put the cursor in the composition box for that fluid and press the Remove Fluid button. You will be prompted for confirmation before the fluid is removed.

The Copy button places the fluid names and compositions (separated by tabs) onto the clipboard so that they can be pasted into other applications. The Paste button will paste the values that are on the clipboard into the composition boxes.   The paste function is smart enough to search through multiple columns in the information stored on the clipboard for a column that contains numbers that sum to 1. For example, the copy button pastes both the fluid names and compositions to the clipboard. If the paste button is then pressed, the program realizes that the first column does not contain compositions and will paste the second column into the composition boxes.
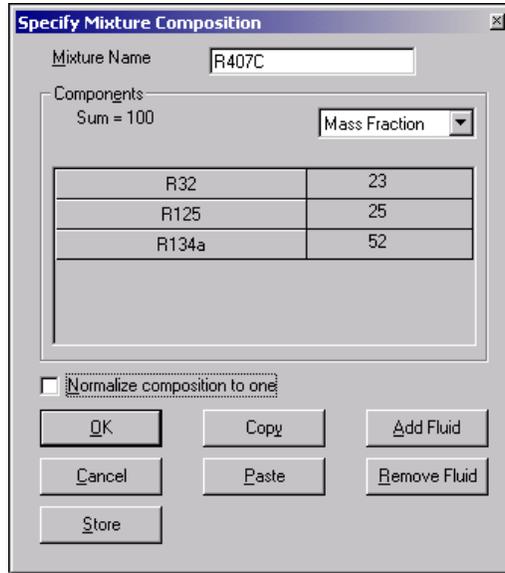
4.4.2 Storing a mixture for future use

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.

4.4.3 Specifying a fluid set

With the increase in the number of fluids contained in REFPROP, it is often desirable to select only a certain number of fluids that you are interested in. This is done through the Specify Fluid Set dialog. Four default sets are available, and can be changed by the user to match their own preferences. To use one of the four sets, simply click on it and press OK.
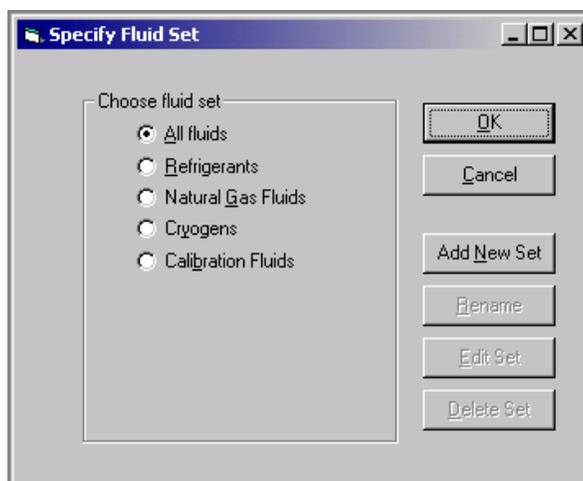
To enter a new set, press the Add New Set button and enter a descriptive name. The Rename button allows you to rename a file set, and the Delete Set button allows you to delete the set. To specify which fluids are in the set, press the Edit Set button and enter/delete fluids in a manner similar to that in the Define New Mixture dialog.

The set labeled "calibration fluids" contains those fluids that generally have both high accuracy equations of state and transport equations. The user should consult the Fluid Information screen to determine what the actual uncertainties in the equations are.

The sets are saved to the hard drive once you press OK. There is no need to save the options to keep the changes just made.

4.5 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

4.5.1 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.

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 half of the 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 in the top portion of the dialog. 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. The Copy All button will generate a listing of all information included in the Information Screen. Buttons near the bottom of the info screen call up similar information for each of the property models. Click the OK button to return to the previous window or dialog.

4.5.2 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.

4.5.3 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 significantly from the true mixture critical parameters depending on the system. 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.
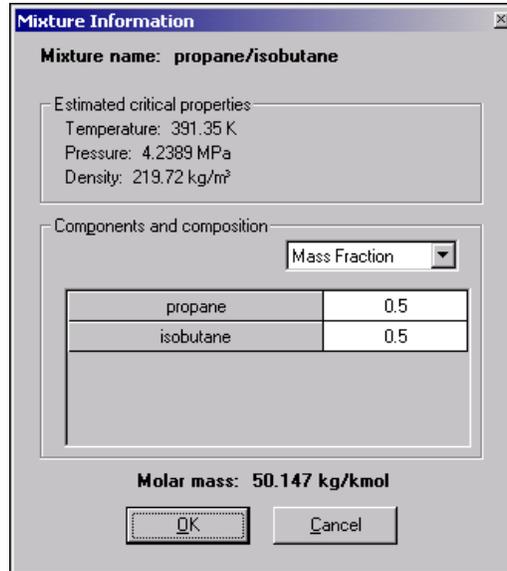
4.6 Viewing Mixture Parameters

The View Mixing Parameters dialog 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 specified.
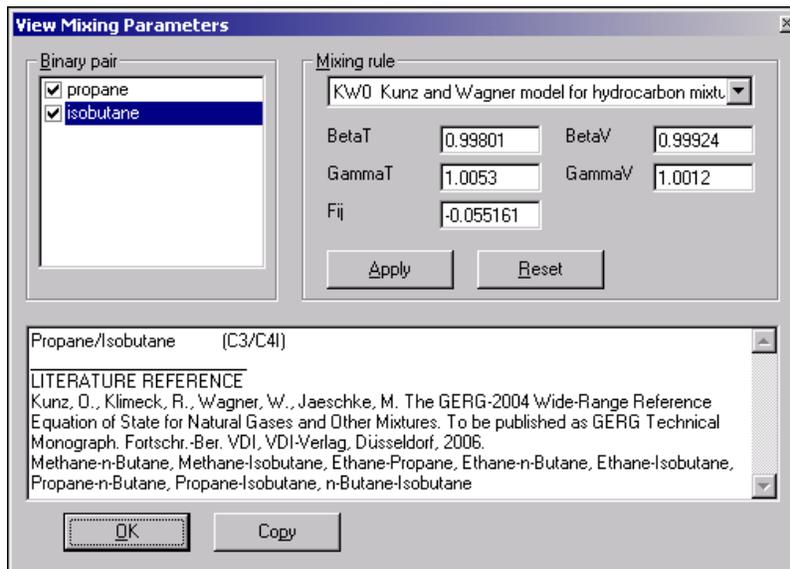
The program calculates mixture properties by applying thermodynamic transformations to the Helmholtz energy. The mixture Helmholtz energy is calculated from the pure-fluid Helmholtz energies through the use of mixing rules. The mixing rules are applied to binary pairs of fluids, so for mixtures with three or more components the binary pair of interest must be specified by clicking the check boxes next to the component names.

The shorthand 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. This information consists of a maximum of 255 characters, due to 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 OK button to return to the main REFPROP window.

4.7 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 values.

Select the binary pair of interest as described in the previous section. 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 and only for the 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 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 spacing of temperature, pressure, density, composition, or quality at some fixed value of another property. The remaining options bring up spreadsheet-type windows that 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.
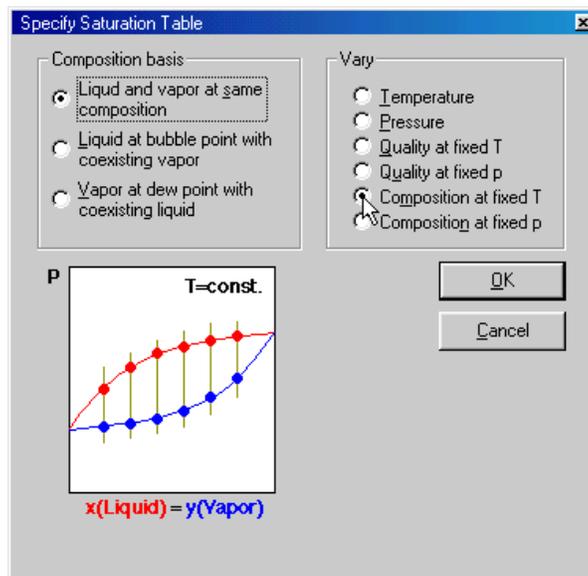
The composition basis for the calculations is specified by the left set of radio buttons. The independent variable is specified by the right set of buttons. Choose one button from each list. A small phase diagram depicts the type of calculation to be performed; this diagram changes as different buttons 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 exercised 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 that have no connection to the composition specified when the system was set up.

For a pure fluid, not all of 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 disabled for fluids lacking equations for the melting and/or sublimation lines.
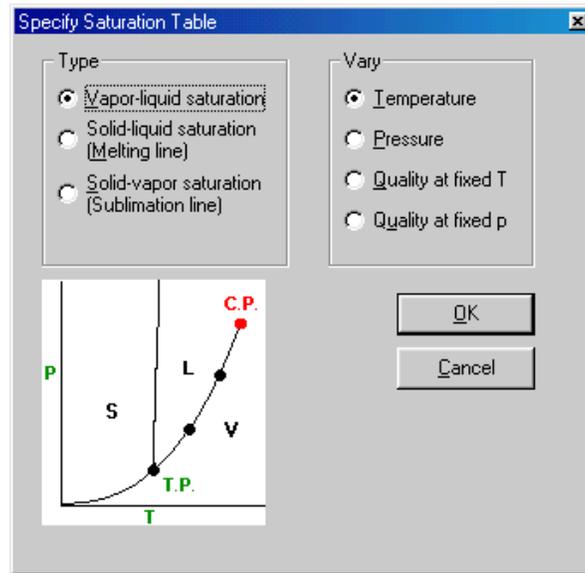
From either the mixture or pure fluid dialog, clicking the OK button brings up a dialog in which the range and increment of the property to be varied and the value of the property to be held constant (if applicable) are entered. Default values are provided. The first time a table is calculated for a 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.
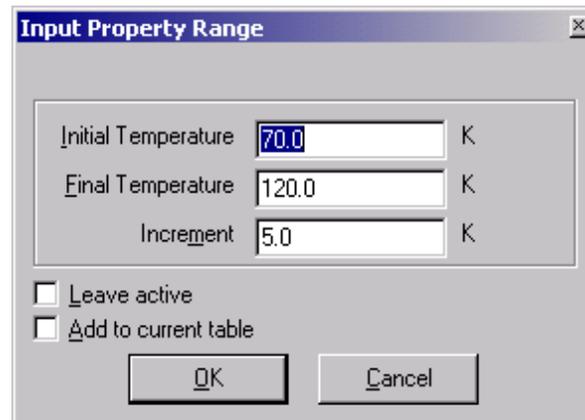
The "Leave active" check box at the lower left keeps this dialog as the top window on the screen, allowing rapid calculation of a series of tables of the same type.

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

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 appears indicating the status. To stop the calculations, click the Cancel button. When the calculations are complete, a table displaying the results appears.

2: propane/isobutane: V/L sat. T=320.0 K: vary composition (0/100)

	Temperature (K)	Liquid Phase Pressure (MPa)	Vapor Phase Pressure (MPa)	Liquid Phase Density (kg/m³)	Vapor Phase Density (kg/m³)	Liquid Phase Enthalpy (kJ/kg)
1	320.00	1.5989	1.5989	454.94	35.742	327.36
2	320.00	1.5099	1.4369	461.97	31.957	325.45
3	320.00	1.4195	1.2980	468.86	28.924	323.76
4	320.00	1.3279	1.1773	475.63	26.424	322.24
5	320.00	1.2349	1.0715	482.32	24.317	320.89
6	320.00	1.1407	0.97770	488.93	22.511	319.65
7	320.00	1.0449	0.89400	495.51	20.941	318.51
8	320.00	0.94729	0.81883	502.06	19.561	317.41
9	320.00	0.84709	0.75096	508.61	18.338	316.32
10	320.00	0.74310	0.68940	515.19	17.248	315.17
11	320.00	0.63335	0.63335	521.81	16.269	313.90

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.
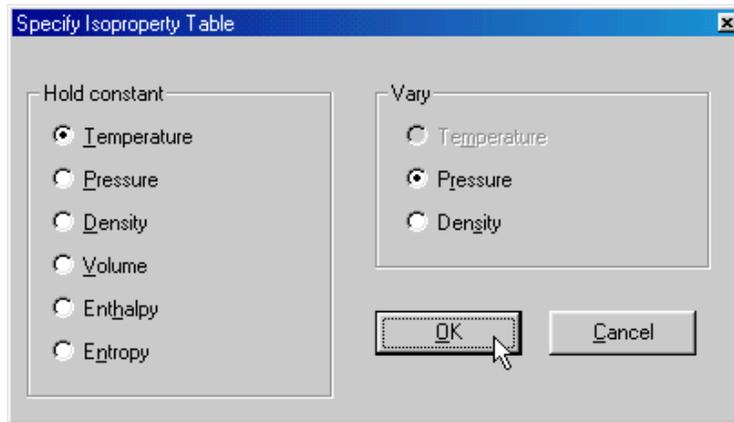
Clicking the OK button brings up a dialog for specifying the value of the property held constant and the range and increment of the varying property; this dialog is similar to that used to calculate saturation tables (see previous section). Default values are provided. The first time a table is calculated 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 the 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). Alternatively, the Add to current table option will add the calculated values for each new isoproperty to the bottom of the current table.

Clicking the OK button initiates the calculations. While the calculations are in progress a small window appears indicating 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.

7: carbon dioxide: T = 20.0 °C

	Temperature (°C)	Pressure (MPa)	Density (kg/m³)	Enthalpy (kJ/kg)	Entropy (kJ/kg-K)
1	20.000	1.0000	19.099	492.53	2.2681
2	20.000	2.0000	40.773	481.32	2.1095
3	20.000	3.0000	66.156	468.46	2.0001
4	20.000	4.0000	97.492	452.99	1.9047
5	20.000	5.0000	140.65	432.38	1.8051
6	20.000	5.7291	194.20	407.87	1.7062
7	20.000	5.7291	773.39	255.87	1.1877
8	20.000	6.0000	782.65	254.28	1.1811
9	20.000	7.0000	808.60	249.95	1.1621
10	20.000	8.0000	827.71	246.91	1.1475
11	20.000	9.0000	843.17	244.58	1.1355
12	20.000	10.000	856.31	242.70	1.1251
13	20.000	11.000	867.81	241.14	1.1158

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.

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

1. Values can simply be 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 Enter, 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 program, select the desired cell in the table and then use 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:

To fill a table with a range of numbers, enter a combination of values into the cells under the "Specify values" section. The value to be placed in the first desired row must be specified in the "First value" field. Beneath this field are additional input boxes in which the last value in the range, the increment (or a multiplier), or last row can be specified. If "Increment" is selected, the value of successive rows in the table is determined by adding the value in the increment field to the previous value. Similarly, if "Multiply" is selected, successive values are determined by multiplying the previous value by the value indicated in the field. If "Last value" is selected, the variable is varied in uniform increments from the specified initial value to the final value. In the special case where you wish to fill a certain number of rows with a constant, enter the starting row, the ending row, and the constant in the "First value" field. The independent values entered must be in the unit system selected with the Units command. You can also specify that the values are saturated liquid or vapor states. This simply adds an "l" or "v" to the number as it places it in the field, as described below.

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.
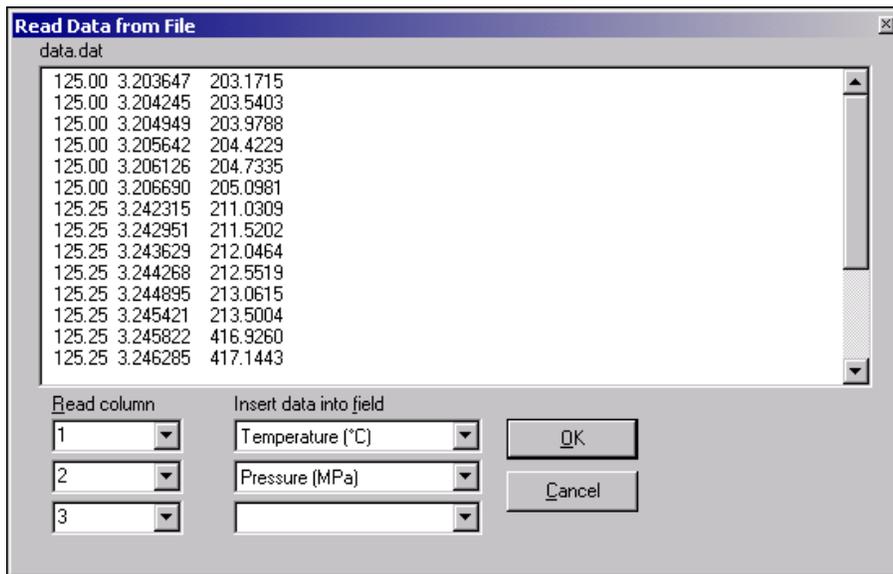
The window displays the first 20 lines of the selected file in the box at the top of the window so that you can see the format of the values in the file. Although only 20 lines are shown, all of the lines are read in when you press the OK button. Lines in the file that begin with a nonnumeric character, such as *, are treated as comments and are ignored. REFPROP will read one or more values from each line in the file and place them in corresponding cells in the blank Specified State Points table.

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.

Extra data from the file can be read and placed in a comment column in the Specified State Points table. The capability to read additional data from a file is useful in comparing experimental and calculated values of a property. Before this can be done, the "Add a comment column to tables" option must be specified in the Preferences dialog (section 7.5), and a new table containing the comment field must be created. The comment field can then be specified in one of the boxes under the "Insert data into field" label. They can then be plotted along with calculated values.

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). The composition fields can be moved permanently in the Property Order menu.

Saturation or melting states can be calculated by adding the letters "l", "v", or "m" before or after the value of temperature, pressure, density, enthalpy, or entropy. Note that "m" returns liquid properties at the solid-liquid boundary. The program does NOT calculate solid properties. In the case where "l" or "v" is entered, and

there is only one valid liquid or vapor state point, that point is returned regardless of whether or not it is in the liquid or vapor state. If a liquid density is entered with a "v", the liquid state is calculated internally; however, the vapor state is returned. The same is true for a vapor state entered with "l". The properties at the critical point can be calculated easily by entering "cr", and the properties at the triple point can be calculated by entering "tr" (liquid properties can be obtained with "trl" and vapor properties with "trv").

For state points that are double valued, the character "<" or ">" can be added to the number (before or after) to find the lower or upper root, respectively. These same characters can also be used to find metastable fluid states for temperature and pressure inputs. For example, the saturation pressure for nitrogen at 100 K is 0.778 MPa. Inputs of 100 K and 0.777 MPa will return a vapor state, but inputs of "100" for temperature and "0.777>" for pressure will return a metastable liquid state.

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 the previous section. 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.

The independent variable(s) can be entered in the same way 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.

When entering temperatures or pressures for mixtures, it is important that the value is placed in the appropriate column. Placing the temperature in the "Liquid phase temperature" column will calculate a bubble point with its corresponding vapor state at some equilibrium condition. Entering the temperature in the

"Vapor phase temperature" column will calculate a dew point with its equilibrium liquid condition. These two lines will be completely different, and can be confusing if the compositions are not displayed.

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.

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. You can 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 in the middle 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 program 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).

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 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. In addition, 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.
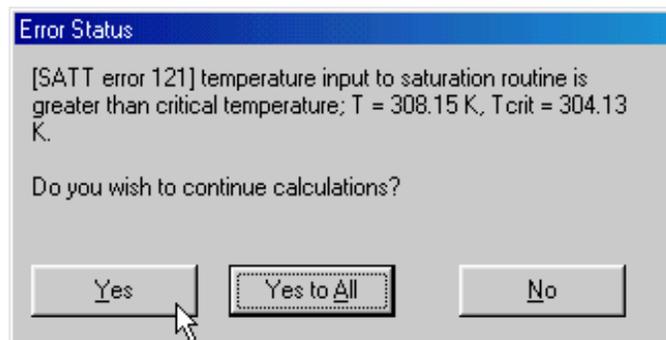
6. CREATING AND MODIFYING PLOTS
(The Plot Menu)

The REFPROP program provides plotting capability for any data appearing in a table. In addition, simple plots of the thermodynamic surface can be easily generated over 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 program is not intended to compete with programs devoted to plotting and data analysis. If you need to produce publication-quality plots or to 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 for transferring 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.
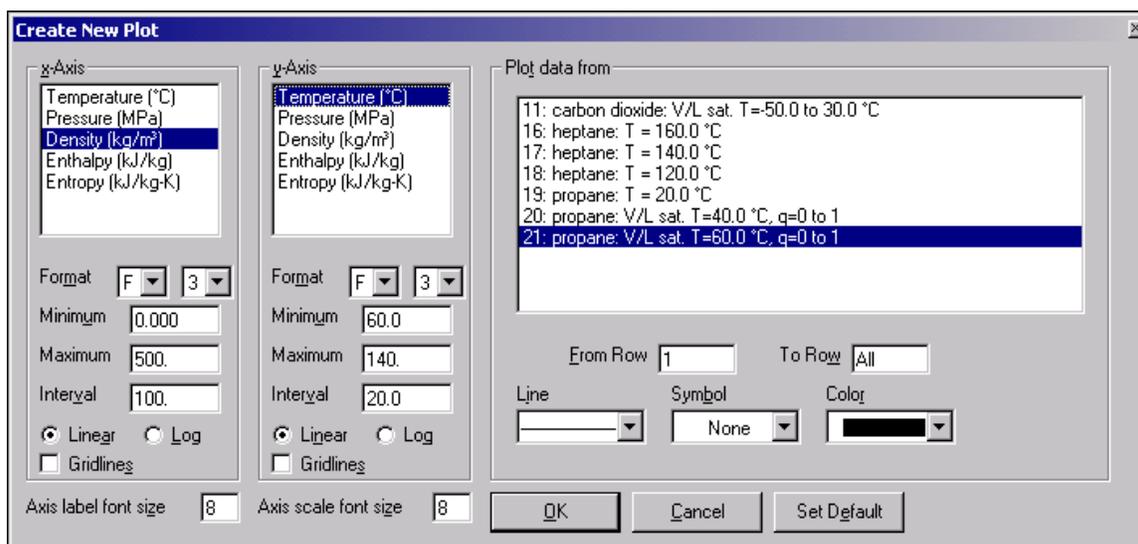
By default, it is assumed that data from the topmost table window are to be plotted. Other tables can be selected using the list at the upper right of the dialog. It is also assumed that all rows in the selected table are to be plotted. If this is not desired the starting and ending row numbers can be entered in the edit boxes below the table list. 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).

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

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 total number of digits (before and 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 options in the lower right portion of the dialog. Points can be connected by a variety of line widths, or no line at all, by selecting the desired option in the drop-down list labeled "Line." The "Symbol" drop-down list provides 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 Set Default 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 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 that 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 program 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
Pressure vs. Temperature
Compressibility Factor vs. Pressure
Enthalpy vs. Entropy
Isochoric Heat Capacity vs. Temperature
Isobaric Heat Capacity vs. Temperature
Speed of Sound vs. Temperature
Exergy vs. Temperature
(Z-1)/density vs. density
Viscosity vs. Temperature
Thermal Conductivity vs. Temperature
Temperature vs. Composition (for binary mixtures only)
Pressure vs. Composition (for binary mixtures only)

Selecting any of these options brings up a dialog in which the properties to be plotted can be specified as shown below.
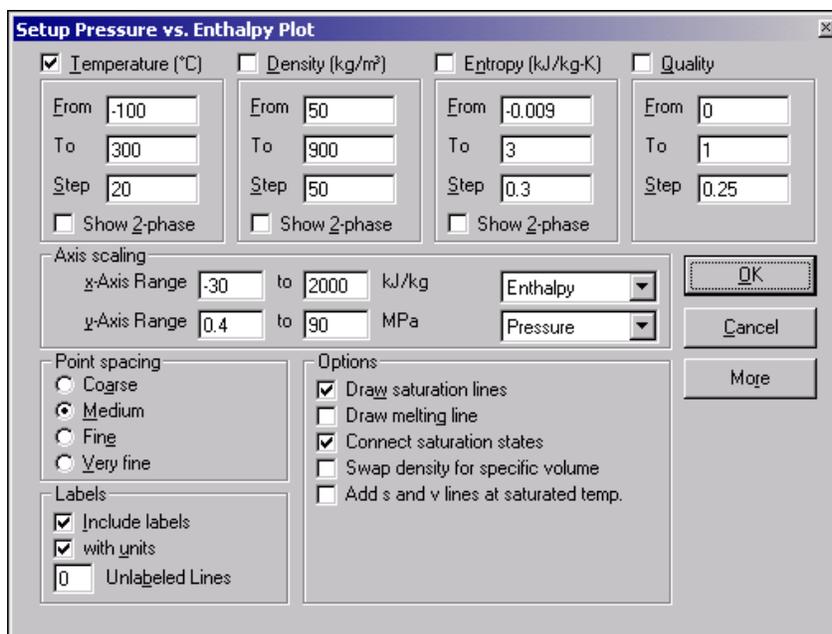
Each diagram type will allow different combinations. In the example shown, a pressure vs. enthalpy diagram can display lines of constant temperature, density, entropy, and/or quality. To plot a property, place a check in the box to the left of the label. You can then specify a range of values to be plotted or up to 12 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.

For cases where multipliers are preferred rather than increments in the "From...To...Step" inputs, the character "*" can be added in front of the step input. Thus, inputs of "From: 0.001, To: 1000, Step: *10" would produce isolines of 0.001, 0.01, 0.1, 1, 10, 100, and 1000. The More/Less button can be selected to include/exclude additional boxes where property values can be individually added.

Labels identifying the isoproperties are automatically generated if the "Include labels" option is selected. You can change or delete these text items or add additional text using the Add Label command. If too many labels are being placed on a plot, the "Unlabeled lines" option can be used to specify that labels should occur on every other line, every third line, and so on. The appearance of the plot can be modified with the Modify Plot command and with the controls in the Plot window.

The amount of data calculated, resulting in fine or coarse plots, can be selected in the "Point spacing" option. Several additional options are available to control whether the saturation lines are drawn, the melting line is drawn, and the saturated liquid and vapor states are connected by lines. The "Swap density for specific volume" option will change the density inputs to volume inputs. The "Add s and v lines at saturated temperature" option will draw a vapor phase isochore and a vapor phase isentrope for each isotherm that is plotted, using the value of volume and entropy at the saturated vapor state point.

In addition, values in the two-phase region can also be plotted with 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 data for metastable states of 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 region.

Other properties can be plotted as well using these same techniques. Under the "Axis" scaling label in the plot dialog, the x and y properties can be changed by selecting the down arrows and clicking on the desired property. Most of the properties available in the Properties dialog can be plotted on the y axis. Properties allowed on the x axis include temperature, pressure, density, volume, energy, enthalpy, entropy, compressibility factor, exergy, -1/T, and composition. In order to avoid problems where one of the four columns at the top of the plot dialog matches one the properties on the x or y axis, you should carefully select as a starting point one of the diagrams in the Plot pull down menu that contains your x or y property. For example, to generate a plot showing the Prandtl number vs. temperature, you could start with a T-s diagram so that the upper four columns show pressure, density, enthalpy, and quality. If a T-h plot was selected, then the third column would contain entropy instead of enthalpy. Once this is done, the x axis property should be changed to temperature and the y axis property should be changed to the Prandtl number. Even better in this case would have been to select a Cv vs. T plot so that temperature is already placed in the x-axis option. Once the initial plot is setup, you can then go to the Plot/Other Diagrams option to modify your previous settings.

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 disabled for pure fluids and for mixtures with three or more components. The picture below displays the output of a T-x plot for R508A.
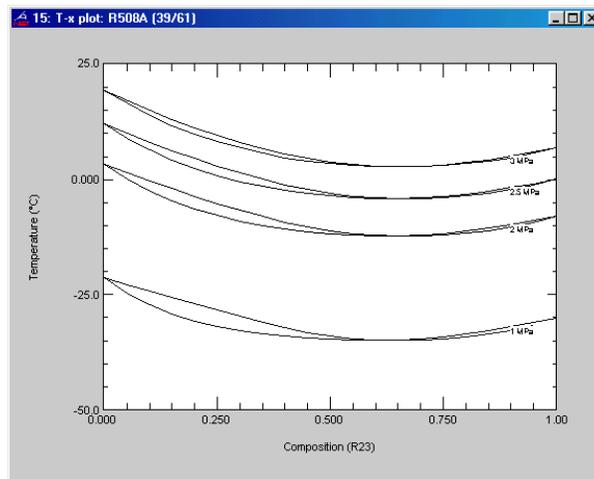
6.4 Modifying Plots

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 are provided below the "X-Axis" and "Y-Axis" portions of the dialog.
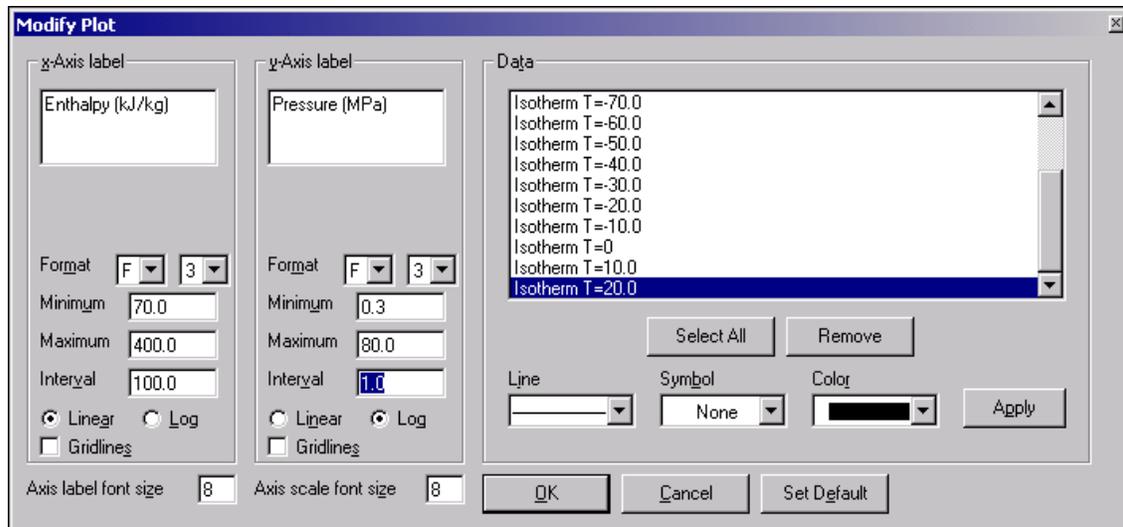
A list box in the upper right lists the individual data sets plotted. Selecting an item allows editing of the line and symbol attributes for that data set. The Remove button permanently deletes the selected data set. (Note that for the predefined plots, there is an entry for each of the lines composing 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.

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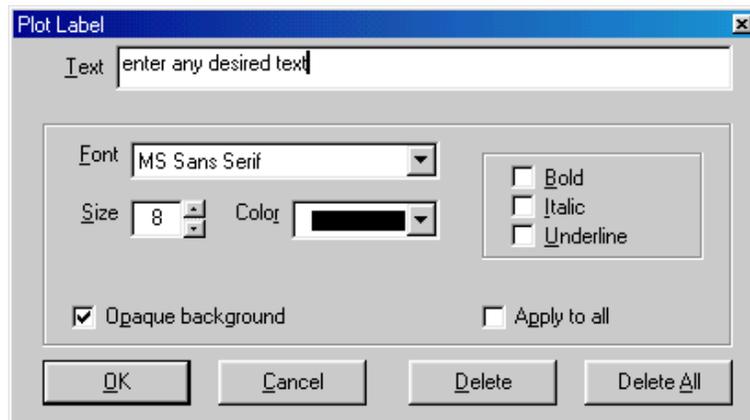
You can modify an existing label (including those generated through the predefined plots) by double-clicking within the boundaries of the text. A label can be permanently deleted with the Delete button. The Delete All button deletes all the labels on a plot.

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

The degree character can be entered into the text of the label by pressing Alt-248 (or Alt-0176) on the numeric keypad. Alt-253 will add a superscript "2" to the text. In addition, Alt-0178 will add a superscript "2"

and Alt-0179 will add a superscript "3". Other special characters of interest using the Alt key include 225: ß, 230 (or 0181): µ, 241 (or 0177): ±, and 246: ÷.

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 location 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.

6.4.6 Add a point to a table

When the right mouse button is clicked within the plotting area, the spot will be marked with a circle, and the values of the properties at the selected state point will appear on the most recently used table (created from Calculate/Specified State Points). If no table is active, the right mouse button marks the spot with a circle only. Points added to the plot in this fashion can then be connected with lines or deleted by entering the Modify Plot option.

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.

Multiple buttons are available for selecting default sets of unit; for example, standard SI or English units. Other sets include standard SI units with Celsius for temperature, a mixed set of SI and English units, and an option to use unitless dimensions for some variables, including temperature divided by the critical temperature, pressure divided by the critical pressure, and so on. 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 molar and mass bases govern the selection in the Mass list box. For example, selecting "kg; kmol" specifies kilograms if the mass basis is selected and 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. This allows you, for example, to specify a mixture composition on a mole fraction basis and display the properties on a mass basis.

Pressures can be expressed as gage pressures by selecting the "Use Gage Pressure" option. The atmospheric pressure or elevation at the location of interest is required to use this option.

7.2 Enthalpy and Entropy Reference States and Exergy

When large differences in enthalpy and entropy occur between REFPROP and tables of properties given in handbooks, please note:

The absolute values of enthalpy, entropy, and energy at a single state point are meaningless. It is only the difference between two different state points that matter. Thus, the value for a single state point can be set to any arbitrary value. Many handbooks set the arbitrary state point so that the values of these properties are positive for most liquid or gas states. You can change the values of the arbitrary state points by going to the Options/Reference State menu. Your choice of options can be permanently saved in the graphical interface by selecting Options/Save Options, and then saving the options under the file name "defaults.prf".

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:

1. The "normal boiling point" (NBP) choice sets the enthalpy and entropy to zero for the 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.

Some 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 differ from the selected convention by amounts equal to the enthalpy and entropy of mixing. This option is convenient when working with a refrigerant blend of specified composition.

The reference state dialog also specifies the conventions used for exergy. Exergy is a specialized property that 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 then be 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 that 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.
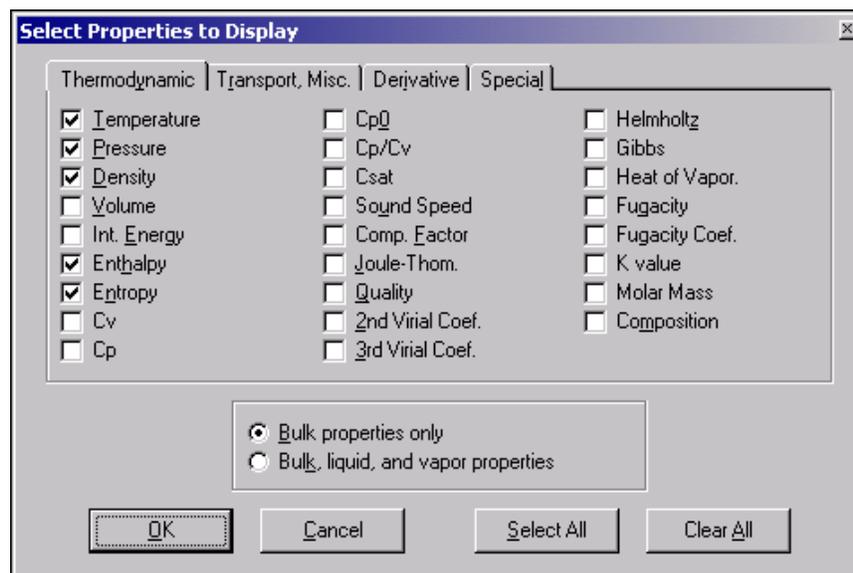
In the lower part of the dialog, a pair of radio buttons controls whether properties for the liquid and vapor phases are to be displayed in addition to bulk properties. Liquid-phase properties are denoted by "Liquid" or "Liquid phase" in the table heading; "Vapor" or "Vapor phase" denotes the vapor-phase 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. 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.)

Most thermodynamic and transport properties can be calculated. The properties that can be displayed are divided into four categories: thermodynamic properties, transport properties plus surface tension and dielectric constant, derivatives of the thermodynamic properties including isothermal compressibility and volume expansivity, and special properties.

Thermodynamic properties include temperature (T), pressure (p), density (D), volume (V), internal energy (e), enthalpy (h), entropy (s), isochoric (Cv) and isobaric (Cp) heat capacities, ideal gas isobaric heat capacity

(Cp0), ratio of Cp to Cv, speed of sound (w), compressibility factor (Z=p/DRT), Joule-Thomson coefficient (JT=dT/dp at constant h), quality (q=ratio of vapor moles to total moles), 2nd virial coefficient (B), and 3rd virial coefficient (C). Most of these properties are given on a molar or mass basis, e.g., V=volume/number of moles. Other properties used more in the chemical industry include the Helmholtz energy (a), Gibbs energy (g), heat of vaporization (hvap), fugacity (f), fugacity coefficients [f_i/x_ip], K value (the ratio of the vapor mole fraction to the liquid mole fraction), molar mass (molecular weight), and composition (on either a mole basis or mass basis).

The transport properties include the thermal conductivity (ThC), viscosity (Vis), kinematic viscosity (Vis/D), thermal diffusivity (ThC/D/Cp), and Prandtl number (Vis*Cp/ThC). The surface tension and dielectric constant are included under the transport properties menu.

Derivative thermodynamic properties include the isothermal compressibility [kappa=1/kt/p= -(dV/dp)/V at constant T], volumetric expansivity (also known as the thermal expansion coefficient) [beta=(dV/dT)/V at constant p], isentropic expansion coefficient (k=w^2*D/p=-V/p(dp/dV) at constant s), isothermal expansion coefficient [kt=D/p(dp/dD) at constant T], adiabatic compressibility [betas=1/k/p=-(dV/dp)/V at constant s], adiabatic bulk modulus [Bs=k*p=-V(dp/dV) at constant s], isothermal bulk modulus (Kt=kt*p=-V(dp/dV) at constant T), isothermal throttling coefficient (-JT*Cp = dh/dp at constant T), and Gruneisen value (dpdT*V/Cv at constant V). Additionally, properties contained under the derivative tab include most of the common derivatives of density, pressure, temperature, and enthalpy with each other. The property dp/dT [sat] is the derivative of the vapor pressure with respect to temperature. The property dh/dZ [sat] is the Waring function (as given in Ind. Eng. Chem., 46:762, 1954) and dB/dT is the derivative of the second virial coefficient with respect to temperature (B is only a function of T).

Special properties include negative reciprocal temperature (-1/T), (Z-1) over the density, exergy, specific heat input [V(dh/dV) at constant P], Cv in the two-phase region (Cv2phase) (only calculated for pure fluids), supercompressibility factor (Fpv=square root of the compressibility factor at 60 °F and 14.73 psia divided by the square root of the compressibility factor at T and p), critical flow factor (the normalized sonic mass flux for inviscid, one-dimensional, steady, isentropic flow), and the internal pressure [T(dp/dT)-p at constant D]. The (Z-1)/D values are best viewed in the Diagrams menu and are interesting in that the values at zero density are the second virial coefficients and the slope of the isotherms at zero density are the third virial coefficients. The ideal gas values of density, enthalpy, entropy, Gibbs energy, and Helmholtz energy are also available (note that these are the ideal values at T and p, not the ideal values at zero pressure such as is the case with Cp0).

Within the "Special" properties tab is the ability to calculate values for metastable fluid states (such as a liquid that has been superheated beyond the saturated state). These include pressure, enthalpy, entropy, Helmholtz energy, Gibbs energy, and compressibility factor. For single phase states, the values of these properties will be identical to those calculated under the "Thermodynamic" properties tab. However, in the two-phase region, the values given are the metastable fluid states, or more precisely, the properties calculated from the equation of state at the given temperature and density. The easiest way to generate these values is to calculate an isotherm in the Isoproperty Table command, varying the density. The two-phase pressure for a pure fluid, calculated from the equation of state, can also be viewed by plotting a p-D diagram with the "Show 2 phase" option checked.

7.4 Property Order

The property order dialog, shown below, establishes the order in which the properties are displayed in a table.
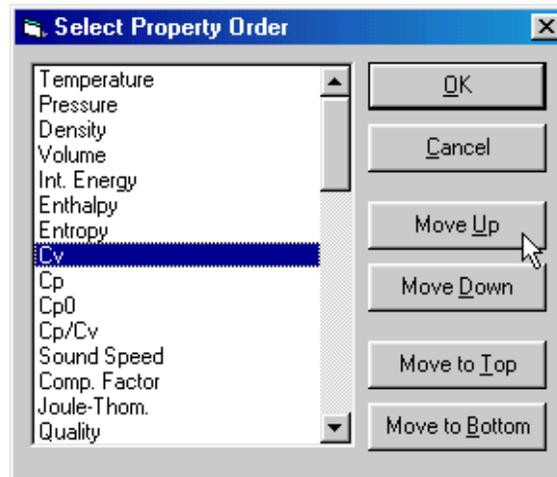
Select the property that you wish to move, and use the "Move up", "Move down", "Move to top," or "Move to bottom" buttons to change the position of that property in any subsequent tables. The property order can also be changed by selecting a property with the up and down arrow keys or the mouse, and 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 program in a number of aspects. Clicking on the check box next to the item activates or deactivates that option.
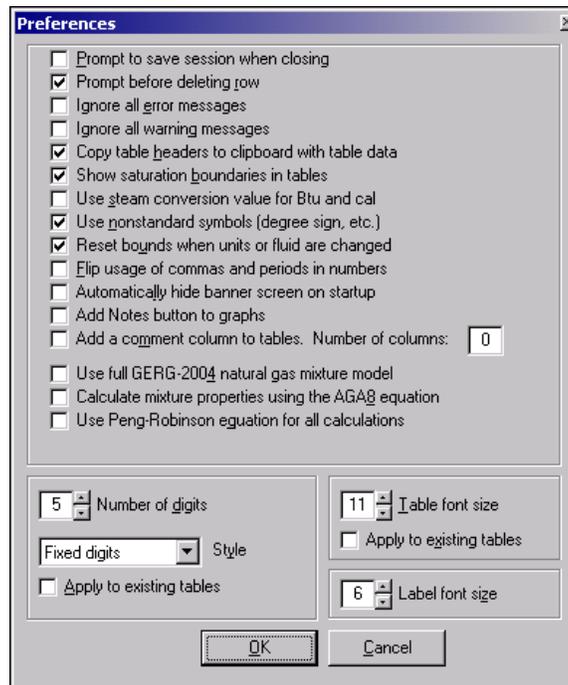
If the "Prompt to save session when closing" option is selected, you will be prompted when the program is terminated to save the session to a file before closing. This file can then be retrieved by selecting the Open Session command (Section 8.2) when the program is run again.

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). Note that a row cannot be recovered after it has been deleted.

The "Ignore all error messages" option will cause all error messages that occur during property calculations to be ignored. 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 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 latter 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 may not be properly displayed, causing unit conversions not to 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 want 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 user's system settings, and this option will not be required.

The "Add Notes button to graphs" option will add a small command button in the upper left corner of each plot that allows the user to add notes to a particular graph. These notes will be printed out under the plot when File/Print is selected. If this option is deselected, the notes that correspond to each plot will not be lost, but will not be accessible.

The option to add a comment column to tables will add one or more extra columns (up to 10) in each table. The extra column(s) 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. 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 mixture model used in REFPROP varies by type of mixture (i.e., refrigerant vs. hydrocarbon mixtures). Constituents typically found in natural gas are modeled by the latest GERG model (finished in 2004). The documentation for this model is still under review. Although the mixing part of the model is similar to that used for the refrigerant mixtures, the pure fluid equations of state have been shortened and differ from the default equations in REFPROP. The calculations using these shorter equations are somewhat faster than the default equations, but are slightly less accurate. If the user wishes to use the shorter equations specified by the GERG-2004 model, the "Use full GERG-2004 natural gas mixture model" option should be selected. This will result in slightly different values than the default values currently calculated. In either situation, the mixing interaction parameters remain the same.

Calculations from the older American Gas Association program for natural gas mixtures can also be made by selecting the "Calculate mixture properties using the AGA8 equation". This equation is not valid in the liquid phase or in the extended region near the critical point and users of this model should be aware of the

uncertainties in the equation in the various regions where they calculate numbers. The default equations in REFPROP are used to calculate the phase boundaries since the AGA8 model does not allow this calculation.

The "Use Peng-Robinson equation for all calculations" option switches from the default equations to the less accurate Peng-Robinson equation. This equation is not recommended for general use in REFPROP.

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 Reformatting 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. An edit box below the style can be used to select the desired number of digits, or the small up or down arrows can be used 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. 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.

The program 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). If you inadvertently 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. Be careful not to confuse any "filename.prf" file with a "filename.rfp" file (a REFPROP session file).

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 program 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 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 program.

The Close command closes all table and plot windows currently on the screen, but the program 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 command. This command, combined with the Save command, 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 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 tables and plot windows 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 save the current work first.

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.
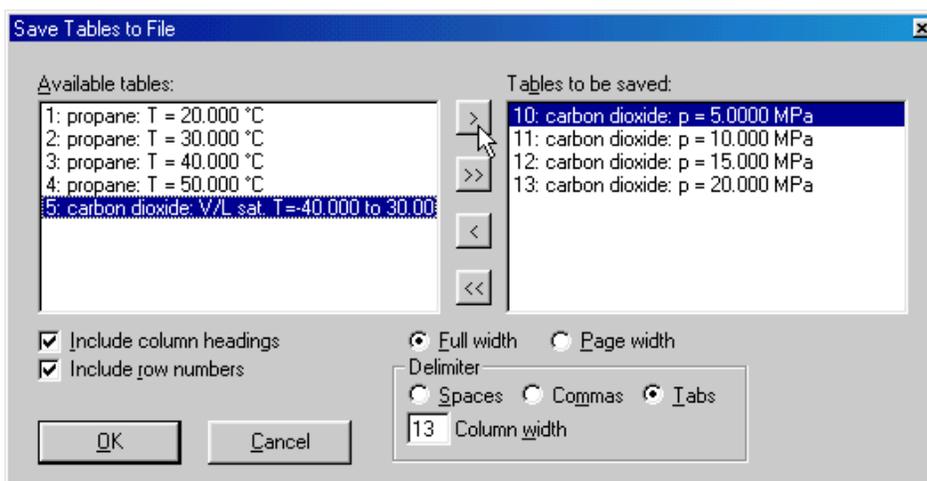
The check boxes at the lower left provide the option to include the column heading (consisting of the property and units on separate lines) and/or the row numbers together with the data. A delimiter selected by the radio buttons at the lower right is placed between each value in a row. Most spreadsheet programs use the tab

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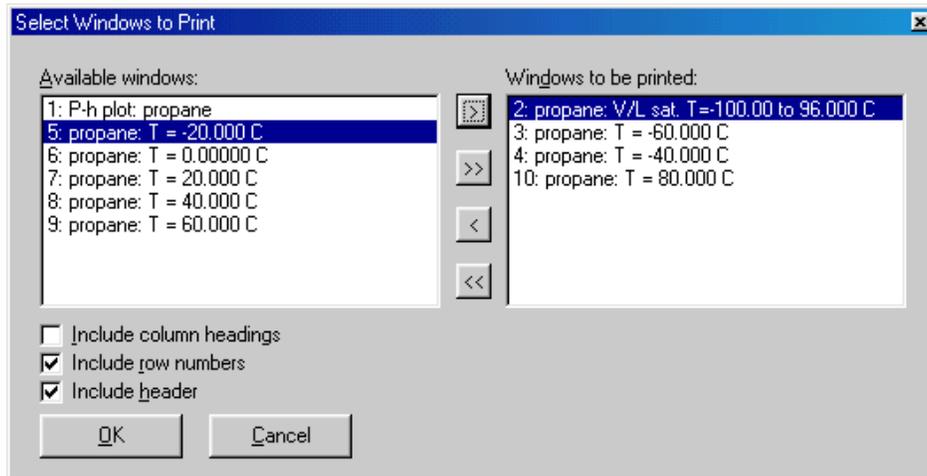
The check boxes at the lower left allow you to include the column headings (containing the property names and units) and/or the row numbers on the printed output of tables. The "Include header" check box will also print out the window header containing the date, time, etc. Multiple tables or plots are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

The Print Dialog command allows for a few additional options while printing, most important is the "Print to file" option. This option sends the output to a file that can then be used in such applications as making PDFs. Unlike the Print Setup command, the Print Dialog command first displays the menu for selecting tables or plots to print, then activates the dialog menu before printing.

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 select the entire table by choosing the Select All command under the Edit menu. The Copy All Table Data command copies all of the information in a table to the clipboard.

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.

The Save Plot Data Points command will save to a file all of the data points used in generating a plot. The first column is the x-axis value, the second column is the y-axis value, and the third column indicates whether or not to connect the point with the previous one. This command is not intended for general use.

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 Inserting and Deleting a Row of Data

The Insert Row command inserts a blank row into the current table where the cursor is located.   The Delete Row command allows a specified row to be permanently removed from the table. In both cases, the rows are not renumbered. These commands are accessible only if a window displaying a table is active. 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 Renaming 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.
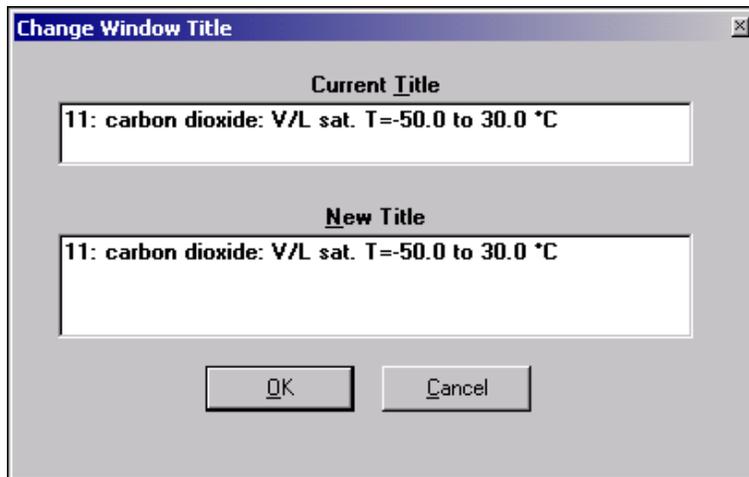
10.3 Going to a Window

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 HELP SYSTEM
(The Help Menu)

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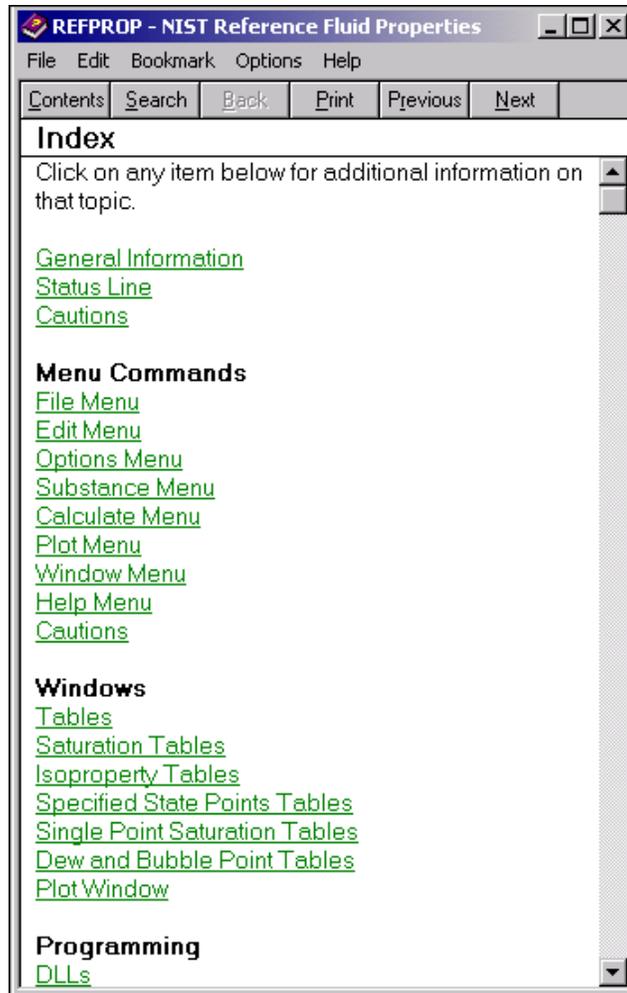
A search capability is available by pressing the Search button. The previous topic is recalled by pressing the Back button. The History button (which is accessed from the Help Options menu) lists, and provides access to, the last several topics viewed.

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

Appendix A
FLUIDS IN THE REFPROP DATABASE

Short Name	File Name	CAS number	Full Chemical Name	EOS Temperature and Pressure Limits
acetone	acetone.fld	67-64-1	propanone	178.5-550 K, 700 MPa
ammonia	ammonia.fld	7664-41-7	ammonia	195.495-700 K, 1000 MPa
argon	argon.fld	7440-37-1	argon	83.8058-2000 K, 1000 MPa
benzene	benzene.fld	71-43-2	benzene	278.7-635 K, 78 MPa
butane	butane.fld	106-97-8	n-butane	134.895-575 K, 69 MPa
butene	1butene.fld	106-98-9	1-butene	87.8-525 K, 70 MPa
carbon dioxide	co2.fld	124-38-9	carbon dioxide	216.592-2000 K, 800 MPa
carbon monoxide	co.fld	630-08-0	carbon monoxide	68.16-500 K, 100 MPa
carbonyl sulfide	cos.fld	463-58-1	carbon oxide sulfide	134.3-650 K, 50 MPa
cis-butene	c2butene.fld	590-18-1	cis-2-butene	134.3-525 K, 50 MPa
cyclohexane	cyclohex.fld	110-82-7	cyclohexane	279.47-700 K, 80 MPa
cyclopropane	cyclopro.fld	75-19-4	cyclopropane	273-473 K, 28 MPa
decane	decane.fld	124-18-5	decane	243.5-675 K, 800 MPa
deuterium	d2.fld	7782-39-0	deuterium	18.71-423 K, 320 MPa
dimethylether	dme.fld	115-10-6	ethylene oxide	131.65-525 K, 40 MPa
dodecane	c12.fld	112-40-3	dodecane	263.6-700 K, 700 MPa
ethane	ethane.fld	74-84-0	ethane	90.368-675 K, 900 MPa
ethanol	ethanol.fld	64-17-5	ethyl alcohol	250-650 K, 280 MPa
ethylene	ethylene.fld	74-85-1	ethene	103.986-450 K, 300 MPa
fluorine	fluorine.fld	7782-41-4	fluorine	53.4811-300 K, 20 MPa
heavy water	d2o.fld	7789-20-0	deuterium oxide	276.97-800 K, 100 MPa
helium	helium.fld	7440-59-7	helium-4	2.1768-1500 K, 100 MPa
heptane	heptane.fld	142-82-5	heptane	182.55-600 K, 100 MPa
hexane	hexane.fld	110-54-3	hexane	177.83-600 K, 100 MPa
hydrogen (normal)	hydrogen.fld	1333-74-0	hydrogen (normal)	13.957-1000 K, 2000 MPa
hydrogen sulfide	h2s.fld	7783-06-4	hydrogen sulfide	187.7-760 K, 170 MPa
isobutane	isobutan.fld	75-28-5	2-methylpropane	113.73-575 K, 35 MPa
isobutene	ibutene.fld	115-11-7	2-methyl-1-propene	132.4-550 K, 50 MPa
isohexane	ihexane.fld	107-83-5	2-methylpentane	119.6-550 K, 1000 MPa
isopentane	ipentane.fld	78-78-4	2-methylbutane	112.65-500 K, 1000 MPa
krypton	krypton.fld	7439-90-9	krypton	115.775-750 K, 200 MPa
methane	methane.fld	74-82-8	methane	90.6941-625 K, 1000 MPa
methanol	methanol.fld	67-56-1	methanol	175.61-620 K, 800 MPa
neon	neon.fld	7440-01-9	neon	24.556-700 K, 700 MPa
neopentane	neopentn.fld	463-82-1	2,2-dimethylpropane	256.6-550 K, 200 MPa
nitrogen	nitrogen.fld	7727-37-9	nitrogen	63.151-2000 K, 2200 MPa
nitrogen triflouride	nf3.fld	7783-54-2	nitrogen trifluoride	85-500 K, 50 MPa
nitrous oxide	n2o.fld	10024-97-2	dinitrogen monoxide	182.33-525 K, 50 MPa
nonane	nonane.fld	111-84-2	nonane	219.7-600 K, 800 MPa
octane	octane.fld	111-65-9	octane	216.37-600 K, 100 MPa
oxygen	oxygen.fld	7782-44-7	oxygen	54.361-2000 K, 82 MPa
parahydrogen	parahyd.fld	1333-74-0p	parahydrogen	13.803-1000 K, 2000 MPa
pentane	pentane.fld	109-66-0	pentane	143.47-600 K, 100 MPa
perfluorobutane	c4f10.fld	355-25-9	decafluorobutane	189-500 K, 30 MPa
perfluoropentane	c5f12.fld	678-26-2	dodecafluoropentane	200-500 K, 30 MPa
propane	propane.fld	74-98-6	propane	85.53-625 K, 1000 MPa
propylene	propylene.fld	115-07-1	propene	87.953-575 K, 1000 MPa
propyne	propyne.fld	74-99-7	propyne	273-474 K, 32 MPa
sulfur dioxide	so2.fld	7446-09-5	sulfur dioxide	197.7-525 K, 35 MPa
sulfur hexafluoride	sf6.fld	2551-62-4	sulfur hexafluoride	223.555-625 K, 150 MPa
toluene	toluene.fld	108-88-3	methylbenzene	178-700 K, 500 MPa
trans-butene	t2butene.fld	624-64-6	trans-2-butene	167.6-525 K, 50 MPa
trifluoroiodomethane	cf3i.fld	2314-97-8	trifluoroiodomethane	120-420 K, 20 MPa
water	water.fld	7732-18-5	water	273.16-2000 K, 1000 MPa
xenon	xenon.fld	7440-63-3	xenon	161.405-750 K, 700 MPa

Short Name	File Name	CAS number	Full Chemical Name	EOS Temperature and Pressure Limits
R11	r11.fld	75-69-4	trichlorofluoromethane	162.68-625 K, 30 MPa
R12	r12.fld	75-71-8	dichlorodifluoromethane	116.099-525 K, 200 MPa
R13	r13.fld	75-72-9	chlorotrifluoromethane	92-403 K, 35 MPa
R14	r14.fld	75-73-0	tetrafluoromethane	120-623 K, 51 MPa
R21	r21.fld	75-43-4	dichlorofluoromethane	200-473 K, 138 MPa
R22	r22.fld	75-45-6	chlorodifluoromethane	115.73-550 K, 60 MPa
R23	r23.fld	75-46-7	trifluoromethane	118.02-475 K, 120 MPa
R32	r32.fld	75-10-5	difluoromethane	136.34-435 K, 70 MPa
R41	r41.fld	593-53-3	fluoromethane	129.82-425 K, 70 MPa
R113	r113.fld	76-13-1	1,1,2-trichloro-1,2,2-trifluoroethane	236.93-525 K, 200 MPa
R114	r114.fld	76-14-2	1,2-dichloro-1,1,2,2-tetrafluoroethane	273.15-507 K, 21 MPa
R115	r115.fld	76-15-3	chloropentafluoroethane	173.75-550 K, 60 MPa
R116	r116.fld	76-16-4	hexafluoroethane	173.1-425 K, 50 MPa
R123	r123.fld	306-83-2	2,2-dichloro-1,1,1-trifluoroethane	166-600 K, 40 MPa
R124	r124.fld	2837-89-0	1-chloro-1,2,2,2-tetrafluoroethane	120-470 K, 40 MPa
R125	r125.fld	354-33-6	pentafluoroethane	172.52-500 K, 60 MPa
R134a	r134a.fld	811-97-2	1,1,1,2-tetrafluoroethane	169.85-455 K, 70 MPa
R141b	r141b.fld	1717-00-6	1,1-dichloro-1-fluoroethane	169.68-500 K, 400 MPa
R142b	r142b.fld	75-68-3	1-chloro-1,1-difluoroethane	142.72-470 K, 60 MPa
R143a	r143a.fld	420-46-2	1,1,1-trifluoroethane	161.34-650 K, 100 MPa
R152a	r152a.fld	75-37-6	1,1-difluoroethane	154.56-500 K, 60 MPa
R218	r218.fld	76-19-7	octafluoropropane	125.45-440 K, 20 MPa
R227ea	r227ea.fld	431-89-0	1,1,1,2,3,3,3-heptafluoropropane	146.35-475 K, 60 MPa
R236ea	r236ea.fld	431-63-0	1,1,1,2,3,3-hexafluoropropane	242-500 K, 60 MPa
R236fa	r236fa.fld	690-39-1	1,1,1,3,3,3-hexafluoropropane	179.52-500 K, 40 MPa
R245ca	r245ca.fld	679-86-7	1,1,2,2,3-pentafluoropropane	200-500 K, 60 MPa
R245fa	r245fa.fld	460-73-1	1,1,1,3,3-pentafluoropropane	171.05-440 K, 200 MPa
R365mfc	r365mfc.fld	406-58-6	1,1,1,3,3-pentafluorobutane	239-500 K, 35 MPa
RC318	rc318.fld	115-25-3	octafluorocyclobutane	233.35-623 K, 60 MPa

PREDEFINED MIXTURES IN THE REFPROP DATABASE

ASHRAE Designation	Components	Composition (mass percentages)	Composition (molar fractions)
air	N2/Ar/O2	75.57/1.27/23.16	0.78120/0.00920/0.20960
R401A	R22/R152a/R124	53/13/34	0.57885/0.18587/0.23527
R401B	R22/R152a/R124	61/11/28	0.65492/0.15461/0.19047
R401C	R22/R152a/R124	33/15/52	0.38559/0.22945/0.38496
R402A	R125/Propane/R22	60/2/38	0.50766/0.04606/0.44628
R402B	R125/Propane/R22	38/2/60	0.29986/0.04296/0.65719
R403A	Propane/R22/R218	5/75/20	0.10430/0.79785/0.09785
R403B	Propane/R22/R218	5/56/39	0.11708/0.66873/0.21418
R404A	R125/R134a/R143a	44/4/52	0.35782/0.03826/0.60392
R405A	R22/R152a/R142b/RC318	45/7/5.5/42.5	0.58240/0.11860/0.06125/0.23776
R406A	R22/Isobutane/R142b	55/4/41	0.57156/0.06184/0.36660
R407A	R32/R125/R134a	20/40/40	0.34642/0.30032/0.35326
R407B	R32/R125/R134a	10/70/20	0.19787/0.60036/0.20177
R407C	R32/R125/R134a	23/25/52	0.38111/0.17956/0.43933
R407D	R32/R125/R134a	15/15/70	0.26227/0.11368/0.62405
R407E	R32/R125/R134a	25/15/60	0.40261/0.10471/0.49268
R408A	R125/R143a/R22	7/46/47	0.05075/0.47628/0.47297
R409A	R22/R124/R142b	60/25/15	0.67609/0.17848/0.14543
R409B	R22/R124/R142b	65/25/10	0.72671/0.17709/0.09620
R410A	R32/R125	50/50	0.69761/0.30239
R410B	R32/R125	45/55	0.65369/0.34631
R411A	Propylene/R22/R152a	1.5/87.5/11	0.02936/0.83347/0.13717
R411B	Propylene/R22/R152a	3/94/3	0.05922/0.90305/0.03773
R412A	R22/R218/R142b	70/5/25	0.74619/0.02451/0.22930
R413A	R218/R134a/Isobutane	9/88/3	0.04976/0.89658/0.05366
R414A	R22/R124/Isobutane/R142b	51/28.5/4/16.5	0.57172/0.20242/0.06671/0.15915
R414B	R22/R124/Isobutane/R142b	50/39/1.5/9.5	0.58744/0.29031/0.02622/0.09603
R415A	R22/R152a	82/18	0.77678/0.22322
R415B	R22/R152a	25/75	0.20295/0.79705
R416A	R134a/R124/Butane	59/39.5/1.5	0.64718/0.32393/0.02888
R417A	R125/R134a/Butane	46.6/50/3.4	0.41446/0.52310/0.06244
R418A	Propane/R22/R152a	1.5/96/2.5	0.02878/0.93920/0.03202
R419A	R125/R134a/DME	77/19/4	0.70146/0.20360/0.09494
R420A	R134a/R142b	88/12	0.87839/0.12161
R421A	R125/R134a	58/42	0.54001/0.45999
R421B	R125/R134a	85/15	0.82810/0.17190
R422A	R125/R134a/Isobutane	85.1/11.5/3.4	0.80550/0.12804/0.06646
R422B	R125/R134a/Isobutane	55/42/3	0.49729/0.44670/0.05601
R422C	R125/R134a/Isobutane	82/15/3	0.77476/0.16671/0.05853
R422D	R125/R134a/Isobutane	65.1/31.5/3.4	0.59629/0.33940/0.06431
R423A	R134a/R227ea	52.5/47.5	0.64812/0.35188
R424A	R125/R134a/Isobutane/Butane/Isopentane	50.5/47.9/1/0.6	0.45615/0.49939/0.01679/0.01865/0.00902
R425A	R32/R134a/R227ea	18.5/69.5/12	0.32113/0.61513/0.06373
R426A	R125/R134a/Butane/Isopentane	5.1/93/1.3/0.6	0.04315/0.92568/0.02272/0.00845
R427A	R32/R125/R143a/R134a	15/25/10/50	0.26078/0.18839/0.10762/0.44321
R428A	R125/R143a/Propane/Isobutane	77.5/20/0.6/1.9	0.69433/0.25589/0.01463/0.03515
R500	R12/R152a	73.8/26.2	0.60610/0.39390
R501	R22/R12	75/25	0.80751/0.19249
R502	R22/R115	48.8/51.2	0.62999/0.37001
R503	R23/R13	40.1/59.9	0.49970/0.50030
R504	R32/R115	48.2/51.8	0.73424/0.26576
R507A	R125/R143a	50/50	0.41184/0.58816
R508A	R23/R116	39/61	0.55758/0.44242
R508B	R23/R116	46/54	0.62675/0.37325
R509A	R22/R218	44/56	0.63079/0.36921

Appendix B

USING REFPROP WITH OTHER PROGRAMS
FORTRAN SOURCE CODE

The subroutines are contained in a number of files, which are placed in the "FORTRAN" directory. The following files 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 core_mlt.for	core_ph0.for	core_pr.for	core_stn.for	
flash2.for flsh_sub.for	idealgas.for	mix_aga8.for	mix_hmx.for	
prop_sub.for	realgas.for	sat_sub.for	setup.for	setup2.for
trns_ecs.for trns_tcx.for	trns_vis.for	trnsp.for	utility.for	

One additional file comes with REFPROP. This file, called pass_ftn.for, is only used when creating the DLL.

Several example files showing how to call the routines are located in your REFPROP\Examples directory. EXAMPLE.FOR shows the common routines that you might need. EX-MIX.FOR shows how to load a mixture .MIX file containing information for specified blends of refrigerants (and air). The file EX-PPF.FOR shows how to use the pseudo-pure fluid files.

Any fluids that are used must have a ".fld" extension, e.g., R134a.fld, or a ".ppf" extension, e.g., air.ppf. 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 subroutines and 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 three standard reference states for entropy and enthalpy and will automatically load the "NIST-recommended" models for the components as well as mixing rules. The routine SETMOD allows the specification of other models. 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 additional routines 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)
```

Subroutine SETUP0 calls subroutine SETUP using the same techniques as those used by the graphical interface and the Excel spreadsheet. Subroutine SETMIX reads the *.MIX files and makes the appropriate call to subroutine SETUP. Subroutine SETPATH sets the path where the *.fld files can be found. Subroutine PUREFLD allows the user to calculate the properties of a pure fluid when a mixture has been loaded and the fluid is one of the constituents in the mixture.

B.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
$d^2(p)/d(rho)^2$	$kPa·(L/mol)^2$
viscosity	$\mu Pa·s \ (10^{-6} \ Pa·s)$
thermal conductivity	W/(m·K)
dipole moment	debye
surface tension	N/m

Note: The only exceptions to the above are the conversion utilities XMASS and XMOLE. The interface allows a wide variety of units, but not the subroutines.

B.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 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.

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

The file MANUAL.TXT located in your REFPROP\FORTRAN directory contains a description of the high-level subroutines that would be used in stand-alone applications. These subroutines will give you access to all features in a model-independent fashion. (There are corresponding low-level subroutines for some of these that 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.)

B.3 Excel Spreadsheets

The REFPROP software includes dynamic link library (".dll") support that allows a broad variety of applications to take advantage of REFPROP's capabilities. REFPROP is distributed with front-end software that links Microsoft Excel applications to fluid property functions.

The REFPROP Excel front-end is supplied as a Microsoft Visual Basic module. Excel automatically incorporates Visual Basic as a macrofunction execution, scripting and interface utility. When the REFPROP front-end module is imported into an Excel spreadsheet, REFPROP functions become accessible to the user.

The information given below demonstrates the front end usage; however, the user is not bound to this format; rather, the preferred method would be to write one's own Visual Basic code that calls the DLL directly. A dedicated module will increase the speed of the application and give the ability to use the REFPROP functions to their fullest.

The following supplementary instructions are intended for users who wish to create and modify their own spreadsheets that utilize the REFPROP functions based on the front-end module. The Excel application included with the software is called REFPROP.xls and is located in the directory where the REFPROP program was installed. Sample FORTRAN and Visual Basic files are also included.

Properties are calculated by calling various functions. 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","SI",300,10)

Other properties can be calculated by using any of the following functions:

Temperature	IsentropicExpansionCoef
Pressure	IsothermalCompressibility
Density	VolumeExpansivity
CompressibilityFactor	AdiabaticCompressibility
LiquidDensity	AdiabaticBulkModulus
VaporDensity	IsothermalExpansionCoef
Volume	IsothermalBulkModulus
Energy	Viscosity
Enthalpy	ThermalConductivity
Entropy	Prandtl
IsochoricHeatCapacity (or Cv)	SurfaceTension
IsobaricHeatCapacity (or Cp)	DielectricConstant
SpeedOfSound (or Sound)	MoleFraction
Quality	MassFraction
HeatOfVaporization (or LatentHeat)	LiquidMoleFraction
JouleThompson	VaporMoleFraction
MolarMass	Mole2Mass
EOSMax	Mass2Mole
EOSMin	

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). Appendix A lists these file names.

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 CONCATENATE 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 stored mixture files (*.MIX) can also be read by simply replacing the fluid name with the name of the mixture file:

    =Enthalpy("R410A.MIX","TD","molar SI",300,5)

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 in which

the properties are sent). Other valid inputs include the density (D), energy (E), enthalpy (H), entropy (S), and quality (Q). Valid combinations include: TP, TD, TH, TS, TE, TQ, PD, PH, PS, PE, PQ, DH, DS, DE, and HS. For saturation states, the second input is Tliq or Tvap for a given saturated temperature, Pliq or Pvap for a given saturated pressure, or Dliq or Dvap for a saturated density. Liquid properties are returned when these inputs contain "liq" and vapor properties are returned when "vap" is used.

The third input to the property functions defines the units. This input can be one of the following: "SI", "SI with C", "Molar SI", "E", "cgs", "mks", "M". If left blank, the default is SI. The "SI with C" input can be shorted to just "C". The units that correspond to these inputs are:

SI: K, MPa, kg/m^3, kJ/kg, kJ/kg-K, m/s, uPa-s, mW/m-K, mN/m
SI with C: C, MPa, kg/m^3, kJ/kg, kJ/kg-K, m/s, uPa-s, mW/m-K, mN/m
Molar SI: K, MPa, mol/dm^3, J/mol, J/mol-K, m/s, uPa-s, mW/m-K, mN/m
mks: K, kPa, kg/m^3, kJ/kg, kJ/kg-K, m/s, uPa-s, W/m-K, mN/m
cgs: K. MPa, g/cm^3, J/g, J/g-K, cm/s, uPa-s, mW/m-K, dyn/cm
E: F, psia, lbm/ft^3, Btu/lbm, Btu/lbm-R, ft/s, lbm/ft-s, Btu/h-ft-F, lbf/ft
M: K, psia, g/cm^3, J/g, J/g-K, m/s, uPa-s, mW/m-K, mN/m

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. This is particularly important when properties for pure fluids that are within the two-phase region are calculated. 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 A5:

=Temperature(A1,"PQ","SI",B1,C1)
=Density(A1,"PQ","SI",B1,C1)
=Energy(A1,"TD","SI",A2,A3)
=Enthalpy(A1,"TD","SI",A2,A3)
=Entropy(A1,"TD","SI",A2,A3)

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 inputs "Tmelt", "Pmelt", "Tsubl", and "Psubl" return melting line or sublimation line values. To calculate the melting pressure for argon at 90 K, enter:

=Pressure("argon","Tmelt","SI",90)

To calculate the melting temperature, enter "Pmelt" as the second input and the melting pressure as the fourth input.

=Temperature("argon","Pmelt","SI",25)

The critical point or triple point is returned in a similar manner via the inputs "crit" or "trip", along with inputs of the fluid name and the units. The molar mass (molecular weight) is returned using the function MolarMass with an input of the fluid name only. All of these functions are shown in the REFPROP.xls file.

REFPROP can be permanently linked to Excel by following these steps:

(This documentation assumes that the REFPROP files have been installed in the "C:\Program Files\REFPROP" directory. Other installations require appropriate adjustments.)

First, execute either step #1 or step #2 (#1 is preferred):

1. An environment variable can be set to specify the locations of the fluid files. This can be done under Start/Settings/Control Panel/System/Advanced/Environment Variables. A new variable called RPPrefix should be created with a value of "C:\Program Files\Refprop" (or the directory where Refprop is located). The environment variable for the path (located under "System variables") can also be modified by adding ";c:\program files\REFPROP" to the end so that the file REFPROP.DLL can be found from any location.

2. From Excel open the file REFPROP.xls located in ...\REFPROP. Open the VB-editor with "Alt-F11". Scroll to the top of the module and read the comments. Make the necessary directory changes as described. The lines should look like this:

.
.
Public Const FluidsDirectory As String = "c:\program files\refprop\fluids\"
Public Const MixturesDirectory As String = "c:\program files\refprop\mixtures\"
.
.

The path marked "c:\..." must point exactly to the location where the REFPROP fluid and mixture files are stored on the user's disk drive. Scroll down several pages and follow the instructions about specifying the path for the Refprop DLL by replacing all occurrences of "Refprop.DLL" with "C:\Program Files\Refprop\Refprop.DLL". Quit the VB-editor and return to Excel and save REFPROP.xls.

3. Save the REFPROP.xls file as a Microsoft Excel Add-In (named REFPROP.xla). The default location will appear as something like ...\Microsoft\AddIns. The file should be saved in this directory. Alternatively, do a search on your computer for the *.xla files and put the REFPROP.xla file in with the others.

4. Open Excel with an empty spreadsheet and find under "Tools" the Add-Ins Manager. Find on the list of available Add-Ins the new entry "REFPROP AddIns". Mark it as active and exit the Add-Ins Manager.

5. Now open any Excel spreadsheet, go to any cell and type something like:

=density("water","TP","SI",500,100)

6. If you need to edit the .xla file after it has been installed, reopen the REFPROP.xls file, edit the VB section, then save it as .xls. Under "Tools" go to the Add-Ins Manager and deselect the REFPROP AddIn. Then save the file again as .xla.

7. Once the module has been imported into a spreadsheet, the REFPROP functions may be selected by using the pull-down function list. When editing the formula in a cell, select More Functions from the pull-down list and scroll down the Function Category list to select the User Defined functions. The argument editor will prompt for REFPROP function arguments as it does for standard Excel functions.

B.4 Visual Basic Applications

Sample Visual Basic (VB) code is provided that demonstrates the use of VB with REFPROP. The file is called Sample.bas and is located in the Examples directory where the REFPROP program was installed. It uses the dynamic link library REFPROP.DLL. Sample FORTRAN and Excel files are also included.

VB subroutines analogous to all of the FORTRAN subroutines 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 because 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 and in the file MANUAL.TXT.

B.5 Sample C Code

The example C code, called EX_C1.CPP (located in the CPP.Zip file), uses explicit (sometimes called late) linking for the functions in the dll. All functions exported by the dll have been provided in the header file, REFPROP1.h, for completeness. All functions exported by REFPROP are in the file PASS_FTN.FOR located the REFPROP\FORTRAN directory. This sample code was tested with the Microsoft Visual C++ compiler in Visual Studio 2003 (Microsoft 32-bit C/C++ Compiler Version 13.10.3077). The main issues in mixed-language code compiling are function naming conventions, argument passing, and stack maintenance. Explicit calling of the FORTRAN functions in the dll allows one to define a function pointer name explicitly. The _stdcall keyword on the function prototype lets the compiler know how arguments will be passed and which side is responsible for cleaning the stack after the function call.

B.6 Sample MATLAB Code

A sample MATLAB file, called refpropm.f90 (located in the MATLAB.Zip file), is available to help software developers link MATLAB with the routines used in REFPROP. The file is located in the directory where the REFPROP program was installed. Sample Visual Basic code and Excel spreadsheets are also included.

The program was written by Lennart Vamling at the Chalmers University of Technology in Sweden and modified by Johannes Lux of the German Aerospace Center and is only intended to show how the calling routines work. To quickly 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 "refpropm.mexw32", "refpropm.m" and the fluid specific files reside.

Otherwise, if the fluids directory is in a different location, one line in the "refpropm.f90" file has to be changed, and 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.

With the \REFPROP\MATLAB directory as the current working directory, issue the following command in MATLAB to reference the REFPROP subroutines:

    mex refpropm.f90 ..\fortran*.for

The REFPROP library for MATLAB was compiled with the version R2006b. Because Mathworks has changed the file extension of external files from .mex to .mexw32 (for 32 bit windows systems), the new interface will not work with MATLAB 6.5. Also, the file refpropm.mexw32 is required to run the interface.

The additional file refpropm.m is only for the help function of MATLAB. If you type "help refpropm", you will see the content of the refpropm.m file.

Some users of the old interface experienced that the first call gave strange answers, but if they repeated exactly the same call, the second gave the correct result. This effect seems to be tied to the 6.5 compiler and is no longer an issue when using the 2006 MATLAB program.

B.7 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) that 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.

Appendix C

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 CDs or installation, please let us know by contacting:

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