

NIST

**REFLEAK:
NIST Leak/Recharge Simulation Model for
Refrigerant Mixtures**

Version 4.0

Users' Guide

David A. Didion
Engineering Laboratory
National Institute of Standards and Technology
Gaithersburg, MD

Min Soo Kim
Seoul National University
Seoul, S. Korea

Piotr A. Domanski
Engineering Laboratory
National Institute of Standards and Technology
Gaithersburg, MD

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1. INTRODUCTION

As alternatives to ozone depleting materials, mixtures of two or more refrigerants are being utilized as working fluids in heat pumping, air conditioning, and refrigeration systems. Generally, these mixtures form zeotropes, which show temperature and composition changes during any evaporation, condensation, or flashing process whether it be intended (i.e., through an expansion device) or unintended such as a leak from a refrigerant container or system. For zeotropic mixtures, it may be important and necessary to predict the composition change for any of these leak conditions.

REFLEAK simulates leak and recharge processes for refrigerant zeotropic mixtures. This Windows-based simulation model provides an easy-to-use package that allows estimation of composition changes of zeotropic mixtures in leak and recharge processes for either vapor or liquid leaks under isothermal or adiabatic conditions. Simulation studies [1, 2] have been carried out and compared to experiments [3, 4].

Thermodynamic properties of the refrigerant mixtures are calculated using the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 9.0 [5]. This Version 4.0 of REFLEAK supersedes Version 3.2, which employed REFPROP Version 8.0. Functional capabilities of Version 3.2 and Version 4.0 are the same.

Uncertainties in Calculated Properties

The 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 temperature and

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pressure. The interested user is referred to REFPROP's original literature sources for details.

The user is further cautioned that, by the very nature of using computational results, 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.

Remarks

Occasionally a convergence problem may occur in calculating thermodynamic properties of some azeotropic or near-azeotropic mixtures. This will result in an error message. Since this will typically occur only for a narrow band of input conditions, the user may want to change the initial input conditions and try the analysis again, or perhaps the property values obtained on either side of the error zone can be interpolated to satisfaction.

NIST regularly updates the REFPROP database [5]. When this occurs, this simulation model will be revised to reflect the new property routines.

This Users' Guide is available for free download at <http://www.nist.gov/srd/nist73.cfm>. In addition to the Users' Guide, the simulation model includes Help Menu with several keywords to assist the user.

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2. INSTALLATION

System Requirements

Free space for complete installation: 10.0 MB
Personal computer (PC) with Microsoft® Windows® 7, XP with Service Pack 3, and Vista operating systems.

The installation module requires .NET Framework 2.0 Service Pack 2 (or later version), which can be downloaded from the Microsoft website if not present on user's PC.

Installation Procedure

Place the REFLEAK CD-ROM in the CD drive. Click [Start], select [Run], type: D:\Setup.exe, or use the appropriate letter associated with the CD-ROM drive, and press [Enter].

Follow the on screen instructions.

3. MODELING OF LEAK AND RECHARGE PROCESS

During a leak process of a refrigerant mixture, fluid in a vapor or liquid phase escapes from the system, where preferential evaporation of one or more components makes the composition in the vapor phase different from that in the liquid phase.

Inherently, the temperature of the fluid in the system decreases since the energy required for vaporization is taken from the refrigerant remaining in the system and from the system wall.

Two idealized cases are considered in the simulation model: (1) isothermal leaks and (2) adiabatic leaks. An isothermal leak process represents a very slow leak situation in which the temperature of the system is maintained constant because of the heat transfer through the walls from the environment. In the adiabatic leak process, it is assumed that the refrigerant leaks so quickly that no heat is transferred through the walls, and thus the temperature in the system decreases as the leak progresses. A comparison of experimental data with REFLEAK simulations has shown that slow leaks are well predicted by the isothermal assumption. However, all real systems have non-negligible heat capacity, which will release some thermal energy during the expanding vaporization process as the liquid temperature drops. Thus, an actual fast leak process probably falls somewhere between the adiabatic and isothermal assumptions.

In order to model these leak situations, the following assumptions are made:

- (1) During the leak, only one phase (vapor or liquid) is escaping from the system.
- (2) The refrigerant mixture inside the system is at a vapor-liquid equilibrium state.
- (3) The leak process is either isothermal or adiabatic.
- (4) The escaping refrigerant has the same composition as the vapor inside the system during the vapor leak, and the same composition as the liquid during the liquid leak.

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In the recharging process, a leak of a portion of the system charge is simulated, and then the system is recharged with a refrigerant of the original composition. The recharged mass is equal to that which has leaked from the system. After recharging during an adiabatic leak process, the temperature in the system is "reset" to the initial temperature.

The leak process is simulated in a quasi-steady manner by alternate steps of refrigerant escaping and adjustment of the remaining refrigerant to thermodynamic equilibrium. The thermodynamic properties are calculated by using the property routines included in the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 9.0 [5]. Therefore, all limitations applicable to REFPROP (e.g., avoiding the region near the critical point) are applicable to REFLEAK.

4. DESCRIPTION OF THE SIMULATION MODEL

The leak/recharge simulation model consists of three parts: (1) a pre-processing section to input required data, (2) a main section to simulate the leak/recharge process, and (3) a post-processing section to display calculated results, and save data and save and/or print graphs.

After initiating the simulation model, a user can take the following actions:

- (1) Selection of the refrigerant mixture for the leak/recharge simulation. Note: the refrigerant mixture must be chosen before any other data can be input or action taken, except that of changing of the units.
 - a. For a predefined blend, press the appropriately labeled command button, use the toolbar, or use the drop down menu: 'Selection/Refrigerants/Predefined Blend'.
 - b. For a user-defined blend press the appropriately labeled command button, use the toolbar, or use the drop down menu: 'Selection/Refrigerants/Define New Blend'.
 - i. Select up to five components from the listbox.

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- ii. Specify the mass (or mole) fractions for each component; in either case, they must sum to one.
 - iii. If desired, the user-defined blend can be stored for later retrieval as a predefined blend.
- (2) Choosing the simulation mode: leak only or leak/recharge.
- (3) Choosing the type of leak: isothermal or adiabatic.
- (4) Choosing the leaking phase: vapor or liquid.
- (5) Choosing of units for temperature, pressure, volume, and mass; (a) units for each may be individually selected or (b) all quantities may be reset to I-P (Inch-Pound) or SI units.
- (6) Inputting the initial leak condition by specifying:
 - a. Initial refrigerant temperature.
 - b. Initial volumetric quality.

Optionally, the initial volumetric quality at the initial temperature can be calculated from a fraction of the maximum liquid fill at a given fill temperature. This option follows the specification of the initial volumetric quality used in ANSI/ASHRAE Standard 34 [6]. Appendix F outlines the calculation procedure used by REFLEAK. Note: if this option is chosen, the user must press the 'Calculate' command button before the 'Analyze' command button will be highlighted and a simulation can proceed.
- (7) Inputting the number of recharge cycles when simulating the leak/recharge process.
- (8) Inputting the mass percentage loss for recharging the system when simulating the leak/recharge process.

After the input data have been specified, click the 'Analyze' command button. After doing so, a DOS window will appear displaying intermediate stages of execution. After the analysis has been completed, a plot window will appear displaying the simulation results.

In the post-processing section, the following functions are provided:

- (1) Displaying of the calculated results in graphical format; the graph shows compositions of the liquid and vapor phases as a function of the leaked mass fraction. A vertical bar in

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the graph indicates specific values corresponding to the x-axis location (leaked mass fraction). The location of the vertical bar can be changed to a specific value of the leaked mass fraction via the slider bar or by typing in the desired value in the data box, both are located in the lower right corner of the screen. Data at this specific value of leaked mass fraction is displayed in the lower part of the graph for temperature, pressure, volumetric quality (void fraction), liquid specific volume, and vapor specific volume. In lieu of compositions of the liquid and vapor phases being plotted along the y-axis, temperature or pressure can be plotted instead using the 'Option' command button and then by using the 'y Data' frame.

- (2) The 'Option' command button can also be used to (i) change the limits of the y-axis by using the 'Limits' frame, (ii) determine whether the liquid and/or vapor phase results will be plotted by using the checkboxes in the 'Show Mass Fractions' frame, and/or (iii) determine the location of the data tags relative to the vertical bar by using the radial buttons in the 'Mass Fractions Display Location' frame.
- (2) Saving output data to a specified file.
- (3) Printing the output data and/or graph.
- (4) Redrawing the graph.
- (5) Closing the display of data and graph.

After a simulation has been completed, another simulation can be executed from the main window. The subsequent simulation can be performed by inputting, if so desired, a different refrigerant mixture and/or different initial conditions, both by repeating the several steps described earlier in this section. If a user selects 'New' from the 'File' menu, all the input data are set to the default values. Note: if the user modifies any of the data after a simulation has been run, the previous simulation results will be removed from memory (the user will be prompted as to whether or not the results should be saved prior to removing them from memory).

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REFERENCES

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<http://fire.nist.gov/bfrlpubs/build95/art090.html>.
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<http://www.nist.gov/srd/nist23.cfm>
- [6] American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc., (ASHRAE), 2004, ANSI/ASHRAE Standard 34-2007, Designation and Safety Classification of Refrigerants".
- [7] McLinden, M.O., 2007, Private communication.

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Appendix A

SAMPLE RUN FOR LEAK PROCESS

A sample execution of the leak/recharge simulation model for a leak process is briefly described below. In this example, a leak process for an R32/134a blend with a composition of 30/70 mass percentage is simulated. The leak process is assumed to be isothermal, and the leaking refrigerant is vapor. The initial temperature is 25 °C, and the initial volumetric quality, which is the ratio of the volume of vapor to the total volume, is 0.25.


To start the simulation model, select the icon 'REFLEAK' in the program window, and then double click the REFLEAK icon.

An introductory screen appears; click the command button 'OK' to proceed.



Figure A-1 Introductory screen

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The main input screen is then displayed (Figure A-2). The first required action is to select the refrigerant. For this example, click the command button 'Define New Blend', after which Figure A-3 will appear. Also, the refrigerant could be specified by using the menu 'Selection/Refrigerants/Define New Blend' or by clicking the toolbar icon .

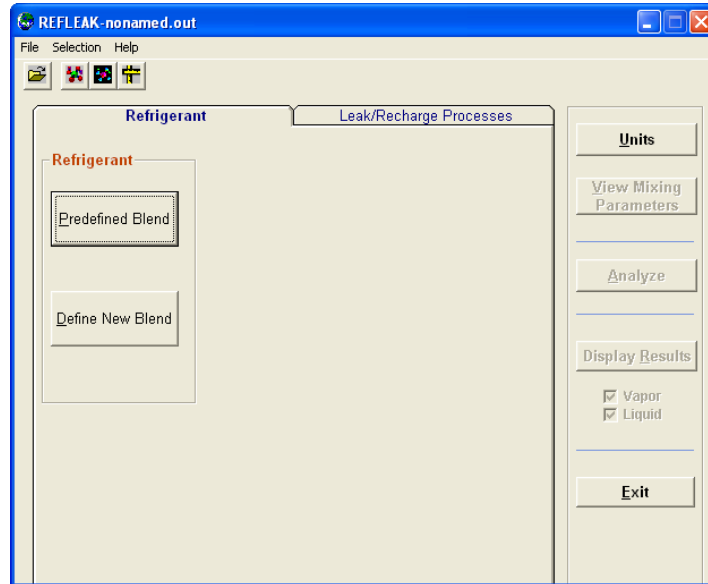


Figure A-2 Main window for data entry

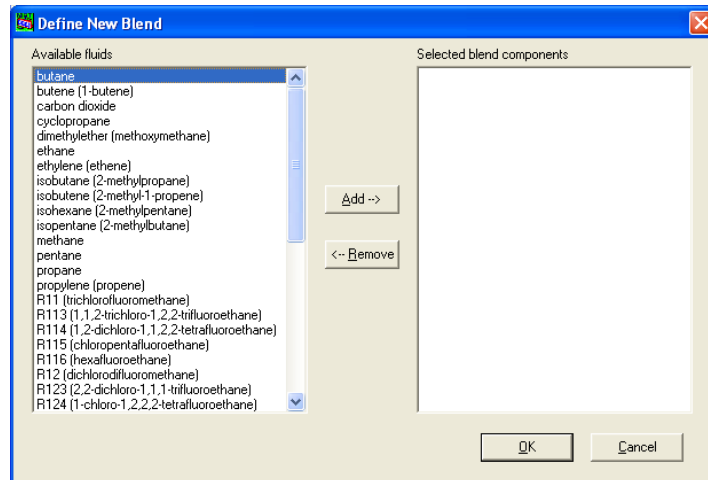


Figure A-3 Refrigerants available for specifying a user-defined blend

For this particular example, first select R32 from the list on the left and click 'Add', and then repeat this action for R134a. After doing so, the window will appear as shown in Figure A-4. Note: to remove a refrigerant from the mixture, select the refrigerant from the list on the right (see Figure A-4) and click 'Remove'. Once the desired refrigerants have been chosen, click 'OK' to proceed to the window shown in Figure A-5. Otherwise, click 'Cancel' and the window shown in Figure A-2 will reappear.

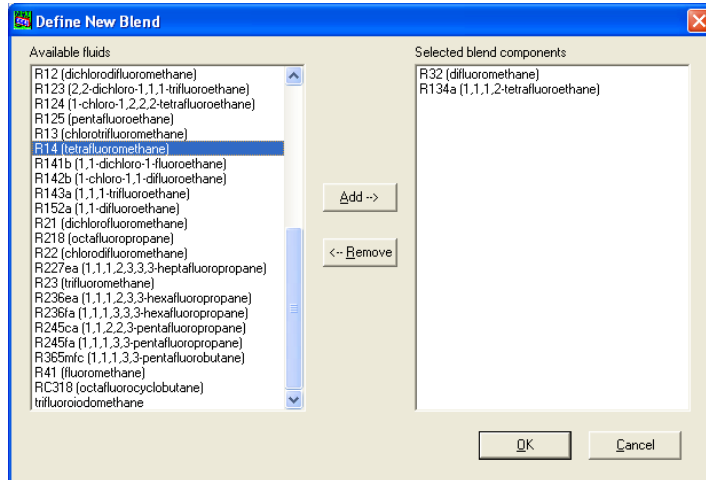


Figure A-4 Appearance of window after selection of refrigerants

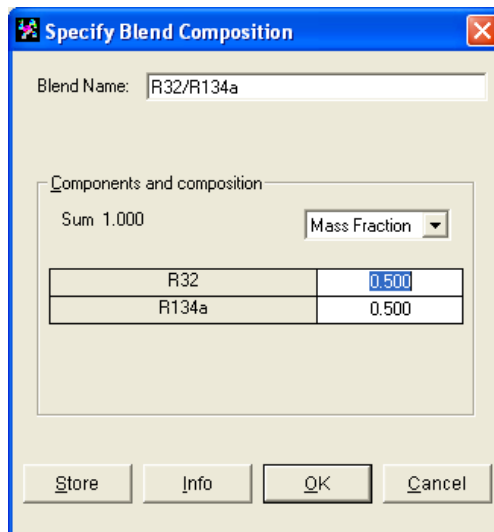


Figure A-5 Window for specifying mixture composition

The specified blend can be stored as a predefined blend by clicking the command button 'Store', after which Figure A-6 will appear. The user can also view basic blend data by clicking the command button 'Info'. To proceed with the previously chosen data, click the command button 'OK', after which Figure A-7 will appear. Otherwise, to annul the selection and return to the original window shown in Figure A-2, click the command button 'Cancel'.

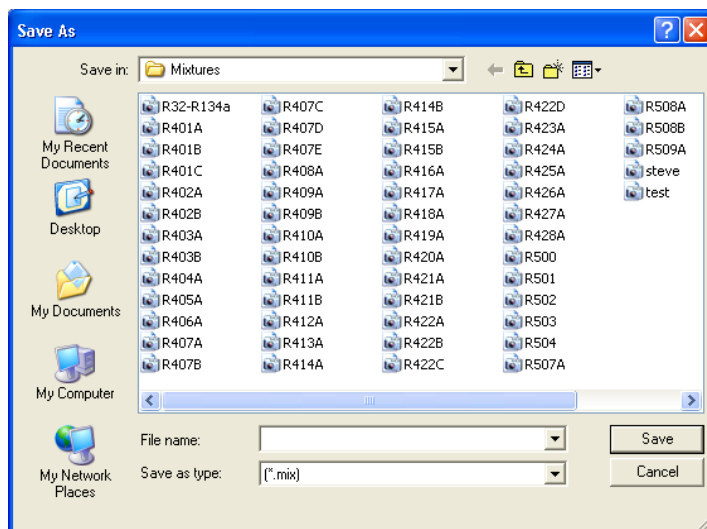


Figure A-6 Storing the user-defined mixture for later use as a predefined blend

The main data entry window (Figure A-7) now provides basic information for the blend, and in addition to the previously enabled command buttons 'Units' and 'Exit', the command buttons 'View Mixing Parameters' and 'Analyze' are now enabled. Also, the checkboxes 'Vapor' and 'Liquid' are now enabled. By alternately clicking one or both of these checkboxes, one can determine if that particular phase will be displayed on the output graph during the post-processing stage.

A simulation can now be initiated using the default initial values by clicking the command button 'Analyze'. If one desires to modify the default initial values, click the tab 'Leak/Recharge Processes', after which Figure A-8 will appear.

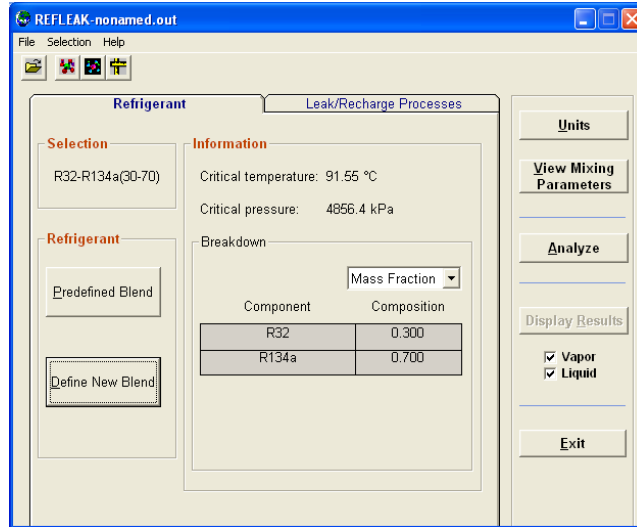


Figure A-7 Main data entry window after specification of mixture

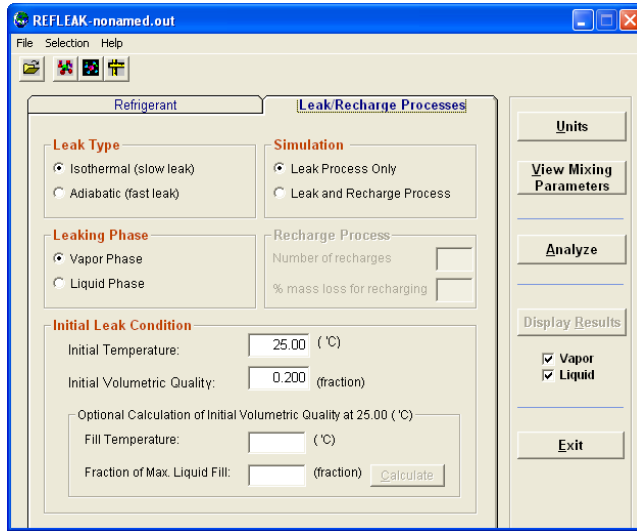


Figure A-8 Main data entry window after clicking 'Leak/Recharge Processes' tab

The default initial values are 25 °C for the initial temperature and 0.2 for the initial volumetric quality. Moreover, the default selections are for an isothermal leak process where the leaking refrigerant is vapor. To modify these selections, click the appropriate radial button, or modify the desired value in the appropriate data boxes. To continue with the example, place the cursor in the 'Initial Volumetric Quality' data box, and enter the value 0.25. If one were to error while typing the input data, a message such as the one shown in Figure A-9 will appear.

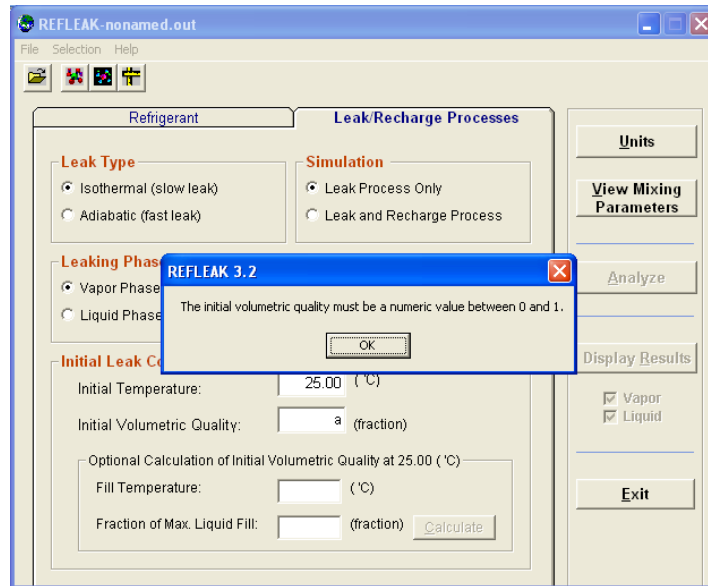


Figure A-9 Sample error message resulting from the mistyping of the input data

Alternately, to implement the optional calculation procedure for the initial volumetric quality, click either the 'Fill Temperature' data box or the 'Fraction of Max. Liquid Fill' data box.

Figure A-10 will then appear. Figure A-10 shows input data for the 'Fill Temperature' and 'Fraction of Max. Liquid Fill', with the 'Calculate' command button enabled. Once the command button 'Calculate' has been clicked, the window shown in Figure A-11 will appear. Now, the 'Analyze' command button is enabled. Note: to once again specify an initial volumetric quality, simply place the cursor in the 'Initial Volumetric Quality' data box. In either case, once data for 'Initial Temperature' and 'Initial Volumetric Quality' are specified, the 'Analyze' command button is enabled.

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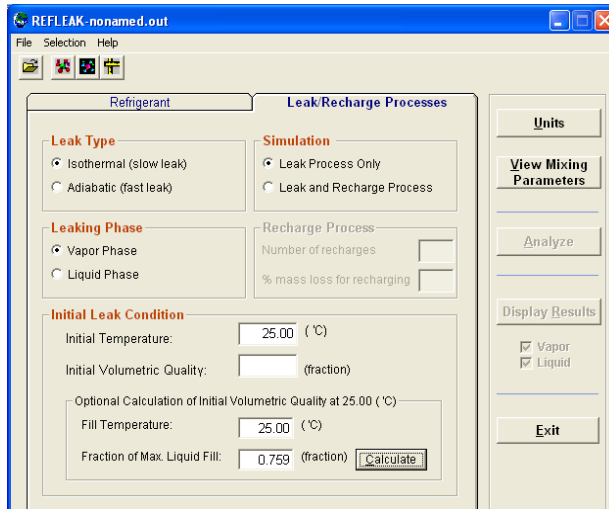


Figure A-10 Input data for optional calculation of the initial volumetric quality

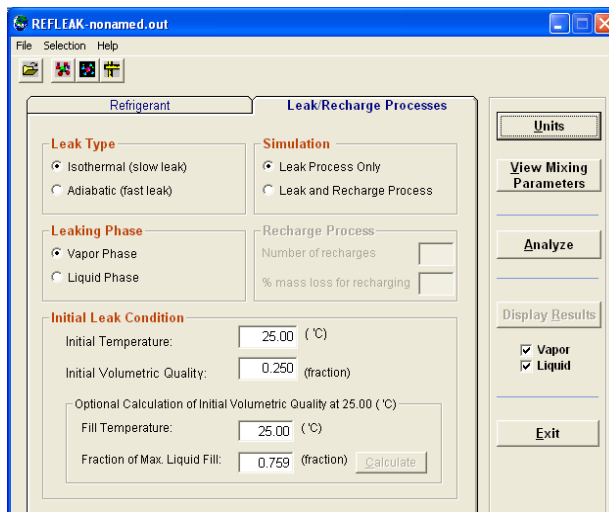


Figure A-11 Input data after 'Calculate' command button has been clicked.

From the main window for data entry (Figure A-2), the user can display the window “Mixing Parameters” (Figure A-12) to view and modify the selection of the mixing rule and mixture parameters used by REFPROP to calculate the thermodynamic properties. The window includes the short-hand name of the mixing rule, the numerical values for the parameters associated with that rule, and reference information. The mixture model is based on pairs of components. For multicomponent mixtures, each binary pair is viewed separately.

Note that changing the mixing rules and mixing parameters is **not intended** for a casual user. The mixing rule and values of mixing parameters displayed in the window – if they have not been altered by the user – are the recommended ones. Great care must be exercised in altering these choices. If the values are modified and the ‘Apply’ command button is clicked, a note “User defined” will be displayed for this particular refrigerant pair.

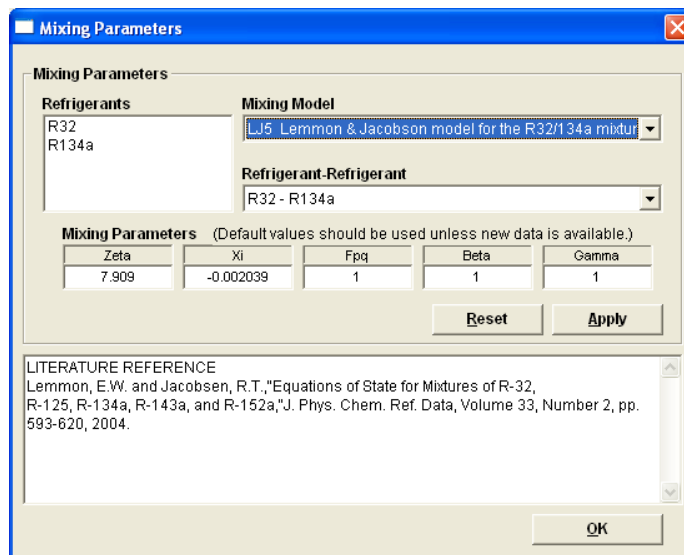


Figure A-12 Window for viewing and changing mixture parameters and mixing rules

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To change the units, click the command button 'Units' on the main window for data entry (Figure A-2). Any combination of the units can be selected individually for temperature, pressure, volume, and mass (Figure A-13). Consistent units can be selected by pressing 'SI' or 'I-P (Inch-Pound)'.

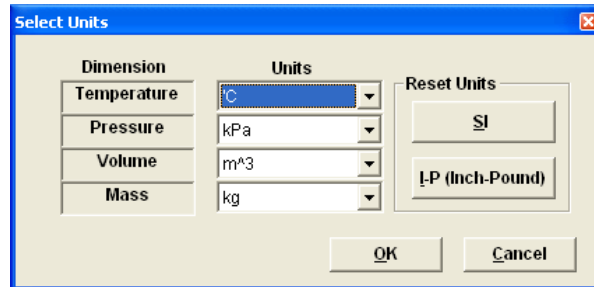


Figure A-13 Selection of units

Click the command button 'Analyze' in the main window to start the simulation.

During model execution, a DOS window appears displaying the simulation progress (Figure A-14). All the calculated data are used for printing and/or plotting purposes.

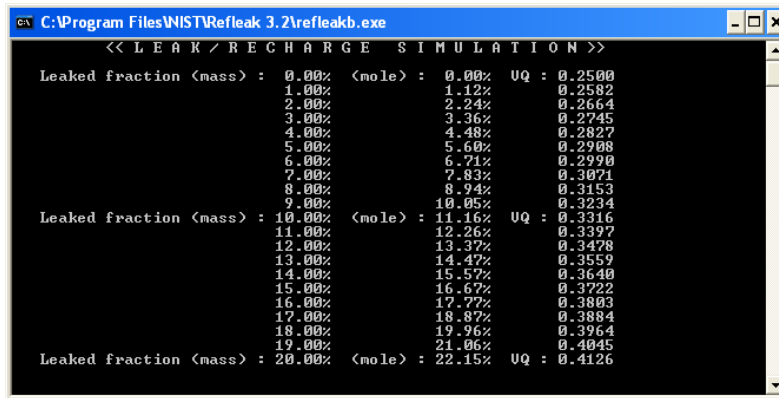


Figure A-14 Progress of simulation for a leak process

After the simulation is complete, a graph (Figure A-15) is displayed showing composition change during the leak or recharge process versus mass percentage leaked out of the system. The vertical bar in the graph indicates the corresponding mass fraction of each of the components. Corresponding vapor and liquid compositions are displayed on the screen as numbers. The vertical bar can be moved by typing x-axis values, or by scrolling the slider located on the lower right. At each mass percentage (x variable), vapor and liquid compositions including temperature, pressure, quality, liquid specific volume, and vapor specific volume are displayed.

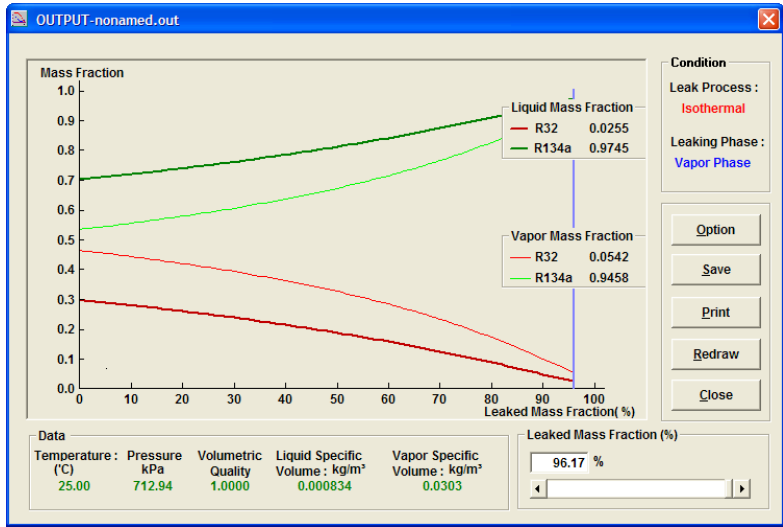


Figure A-15 Data display in a graph format (leak process)

To change the conditions for data display, click the command button 'Option', after which the window shown in Figure A-16 will appear.

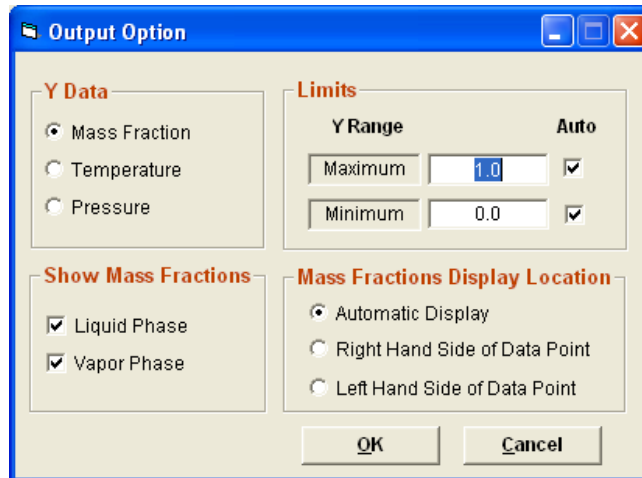




Figure A-16 Options for data display

The data can be saved in a file by clicking the command button 'Save', selecting the menu item 'File/Save', selecting the menu item 'File/Save As', or clicking the toolbar icon .

The data can be printed in tabular or graphical format by clicking the command button 'Print', selecting the menu item 'File/Print', or clicking the toolbar icon .

When the command button 'Redraw' is clicked, the graph is redrawn on the screen, during which time, the command button 'Redraw' is replaced by the command button 'Stop' or by the command button 'Continue'. These can be used to toggle the redrawing process.

Clicking the command button 'Close' reloads the main window.

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Appendix B

SAMPLE RUN FOR LEAK AND RECHARGE PROCESS

This section describes an example of a leak and recharge process. The leak and recharge process for an R32/134a mixture is simulated with an initial composition of 30/70 mass percentage. The leak process is assumed to be isothermal, and the leaking refrigerant is vapor. It is also assumed that the system is recharged when 30 % of the initial mass has leaked out of the system, and that the system is recharged three times with the initial refrigerant composition. The initial temperature is 25 °C, and the initial volumetric quality, which is the ratio of the volume of vapor to the total volume, is 0.25.

Select the icon in the program window, and then double click the REFLEAK icon.

An introductory screen appears (See Figure A-1); click the command button 'OK' to proceed.

Follow the steps in Appendix A to select the refrigerant. Click the tab 'Leak/Recharge Processes' and modify the 'Initial Volumetric Quality' following the steps in Appendix A.

Click the radial button 'Leak and Recharge Process'. Input 3 into the 'Number of recharges' data box, and input 30 in the "% mass loss for recharging" data box, as shown in Figure B-1.

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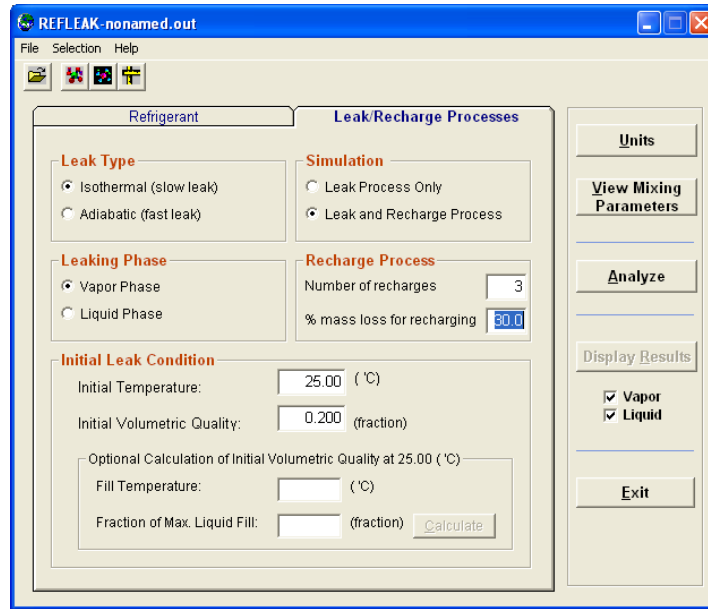


Figure B-1 Data entry window for the leak and recharge simulation example of this Appendix

Click the command button 'Analyze' to start the simulation.

During execution, a DOS window appears to show the progress of the simulation (See Figure B-2).

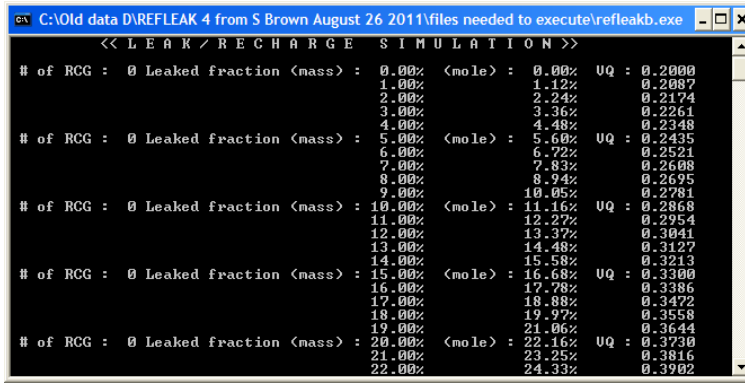


Figure B-2 Window to show progress of simulation (leak and recharge process)

The final output is displayed in graphical format as shown in Figure B-3.

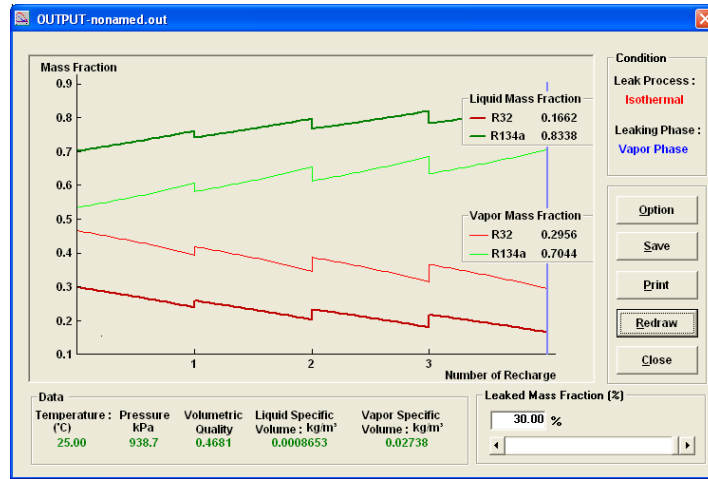









Figure B-3 Data display in graphical format (leak and recharge process)

Appendix C

ICONS

The icons in the tool bar provide additional flexibility and convenience in using REFLEAK. Individual functions and their equivalent menu options are listed below.

<u>Icon</u>	<u>Equivalent File Option</u>	<u>Functions and Uses</u>
	<u>O</u> pen	Open the file saved in a previous process
	<u>S</u> ave	Save the current process
	<u>P</u> rint	Print output
	<u>P</u> redefined Blend	Specify predefined blends
	<u>D</u> efine Blend	Specify user-defined blend
	<u>O</u> utput	Display output
	<u>U</u> nits	Selection of units

Appendix D

SINGLE-COMPONENT REFRIGERANTS AVAILABLE IN REFLEAK

<u>Short Name</u>	<u>Full Chemical Name</u>
R11	trichlorofluoromethane
R113	1,1,2-trichloro-1,2,2-trifluoroethane
R114	1,2-dichloro-1,1,2,2-tetrafluoroethane
R115	chloropentafluoroethane
R116	hexafluoroethane
R1150	ethylene
R12	dichlorodifluoromethane
R123	2,2-dichloro-1,1,1-trifluoroethane
R1234yf	2,3,3,3-tetrafluoroprop-1-ene
R1234ze	trans-1,2,2,2-tetrafluoropropene
R124	1-chloro-1,2,2,2-tetrafluoroethane
R125	pentafluoroethane
R1270 or propylene	propene
R13	chlorotrifluoromethane
R134a	1,1,1,2-tetrafluoroethane
R14	tetrafluoromethane
R141b	1,1-dichloro-1-fluoroethane
R142b	1-chloro-1,1-difluoroethane
R143a	1,1,1-trifluoroethane
R152a	1,1-difluoroethane
R161	fluoroethane
R170	ethane
R21	dichlorofluoromethane
R218	octafluoropropane
R22	chlorodifluoromethane
R227ea	1,1,1,2,3,3,3-heptafluoropropane
R23	trifluoromethane
R236ea	1,1,1,2,3,3-hexafluoropropane
R236fa	1,1,1,3,3,3-hexafluoropropane
R245ca	1,1,2,2,3-pentafluoropropane
R245fa	1,1,1,3,3-pentafluoropropane
R290	propane
R32	difluoromethane
R365mfc	1,1,1,3,3-pentafluorobutane

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<u>Short Name</u>		<u>Full Chemical Name</u>
R41		fluoromethane
R50		methane
R600		butane
R600a	or isobutane	2-methylpropane
R601a	or isopentane	2-methylbutane
R744		carbon dioxide
RC318		octafluorocyclobutane
RE170	or dimethylether (DME)	ethylene oxide
C3H6O		acetone
C6H6		benzene
C4H8		butene
C4H8	or cis-butene	cis-2-butene
C6H12		cyclohexane
C3H6		cyclopropane
C12H26		dodecane
C2H6O	or ethanol	ethyl alcohol
C7H16		heptane
C6H14		hexane
C4H8	or isobutene	2-methyl-1-propene
C6H14	or isohexane	2-methylpentane
C5H12	or isopentane	2-methylbutane
CH3OH		methanol
C5H12	or neopentane	2,2-dimethylpropane
C5H12		pentane
C4H8	or trans-butene	trans-2-butene
CF3I		trifluoroiodomethane
C5F12	or perfluoropentane	dodecafluoropentane
SF6		sulfur hexafluoride

The user can add new fluids to REFLEAK by placing new fluid files into the "fluids" folder. The fluid file must be compatible with REFPROP [5], and its name must start with "R" or "r" (e.g., Rnew2.fld or r754.fld will be recognized by REFLEAK as fluid files).

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Appendix E

PREDEFINED REFRIGERANT MIXTURES AVAILABLE IN REFLEAK

<u>ASHRAE Designation</u>	<u>Composition Components</u>	<u>Mass Percentages</u>
R401A	R22/152a/124	53/13/34
R401B	R22/152a/124	61/11/28
R401C	R22/152a/124	33/15/52
R402A	R125/290/22	60/2/38
R402B	R125/290/22	38/2/60
R403A	R290/22/218	5/75/20
R403B	R290/22/218	5/56/39
R404A	R125/143a/134a	44/52/4
R405A	R22/152a/142b/RC318	45/7/5.5/42.5
R406A	R22/600a/142b	55/4/41
R407A	R32/125/134a	20/40/40
R407B	R32/125/134a	10/70/20
R407C	R32/125/134a	23/25/52
R407D	R32/125/134a	15/15/70
R407E	R32/125/134a	25/15/60
R408A	R125/143a/22	7/46/47
R409A	R22/124/142b	60/25/15
R409B	R22/124/142b	65/25/10
R410A	R32/125	50/50
R410B	R32/125	45/55
R411A	R1270/22/152a	1.5/87.5/11.0
R411B	R1270/22/152a	3/94/3
R412A	R22/218/142b	70/5/25
R413A	R218/143a/600a	9/88/3
R414A	R22/124/600a/142b	51/28.5/4/16.5
R414B	R22/124/600a/142b	50/39/1.5/9.5
R415A	R22/152a	82/18
R415B	R22/152a	25/75
R416A	R124/R134a/600	39.5/59.0/1.5
R417A	R125/134a/600	46.6/50.0/3.4
R418A	R290/22/152a	1.5/96/2.5
R419A	R125/134a/E170	77/19/4
R420A	R134a/142b	88/12
R421A	R125/134a	58/42

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<u>ASHRAE Designation</u>	<u>Composition Components</u>	<u>Mass Percentages</u>
R421B	R125/134a	85/15
R422A	R125/134a/600a	85.1/11.5/3.4
R422B	R125/134a/600a	55/24/3
R422C	R125/134a/600a	82/15/3
R422D	R125/134a/600a	65.1/31.5/3.4
R423A	R134a/227ea	52.5/47.5
R424A	R125/134a/600a/600/C5H12	50.5/47/0.9/1/0.6
R425A	R32/134a/227ea	18.5/69.5/12
R426A	R125/134a/600/C5H12	5.1/93/1.3/0.6
R427A	R32/125/143a/134a	15/25/10/50
R428A	R125/143a/290/600a	77.5/20/0.6/1.9
R429A	DME/152a/600a	60/10/30
R430A	R152a/600a	76/24
R431A	R290/152a	71/29
R432A	R1270/DME	80/20
R433A	R1270/290	30/70
R434A	R125/143a/134a/600a	63.2/18/16/2.8
R435A	DME/152a	80/20
R436A	R290/600a	56/44
R436B	R290/600a	52/48
R437A	R125/134a/600/ C5H12	19.5/78.5/1.4/0.006
R438A	R32/125/134a/600/601a	8.5/45/44.2/1.7/0.6
R500	R12/152a	73.8/26.2
R501	R22/12	75/25
R502	R22/115	48.8/51.2
R503	R23/13	40.1/59.9
R504	R32/115	48.2/51.8
R507A	R125/143a	50/50
R508A	R23/116	39/61
R508B	R23/116	46/54
R509A	R22/218	44/56
R510A	DME/600a	88/12

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Appendix F

CALCULATION OF INITIAL VOLUMETRIC QUALITY BASED ON FRACTION OF MAXIMUM LIQUID FILL

For fractionation analysis, ANSI/ASHRAE Standard 34 [6] specifies a container fill in terms of a “fraction of maximum fill” rather than a vapor volumetric quality. The maximum fill is the calculated mass that gives a 100% liquid fill at the “fill temperature”, which the ASHRAE Standard specifies as 54.4°C (130°F). Note that this temperature may be different than the “initial leak temperature”.

The REFLEAK main input window (Figure A-2) allows the user to use the ASHRAE specification of container fill and to calculate the resulting initial volumetric quality at the initial leak temperature. The following is the calculation procedure used by REFLEAK [7].

Input data:

Original overall (bulk) mixture composition

T_F – liquid fill temperature [K]

F_F – fraction of the maximum liquid fill at T_F [fraction]

T_L – initial leak temperature [K]

Other symbols used:

ρ – density [kg/m^3]

m_{liq} – mass of refrigerant liquid [kg]

m_{vap} – mass of refrigerant vapor [kg]

$xq = m_{\text{vap}} / (m_{\text{vap}} + m_{\text{liq}})$ - vapor quality [kg/kg]

V_{liq} – liquid volume per unit mass of the mixture [m^3/kg]

V_{vap} – vapor volume per unit mass of the mixture [m^3/kg]

$Vq = V_{\text{vap}} / (V_{\text{vap}} + V_{\text{liq}})$ - volumetric quality [m^3/m^3]

Subscripts:

vap – vapor phase

liq – liquid phase

Calculation steps:

1. Calculate the saturated liquid density at T_F and the original mixture composition, $\rho_{liq}(T_F)$
2. Calculate the thermodynamic state point of the mixture defined by:
 - original mixture composition
 - initial leak temperature, T_L
 - filling density of the refrigerant given by $F_F \cdot \rho_{liq}(T_F)$

Results:

- saturated vapor density at the coexisting vapor composition, $\rho_{vap}(T_L)$
- saturated liquid density at the coexisting liquid composition, $\rho_{liq}(T_L)$
- vapor quality, xq

3. Calculate the liquid and vapor volumes per unit mass of the mixture

$$\text{liquid volume: } V_{liq}(T_L) = (1-xq)/\rho_{liq}(T_L)$$
$$\text{vapor volume : } V_{vap}(T_L) = xq/\rho_{vap}(T_L)$$

4. Calculate the volumetric quality, $Vq(T_L)$

$$Vq(T_L) = V_{vap}(T_L)/[V_{vap}(T_L) + V_{liq}(T_L)]$$

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Appendix G

CONTACTS

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

Joan Sauerwein
National Institute of Standards and Technology
Standard Reference Data Group
100 Bureau Drive, Stop 2310
Gaithersburg, MD 20899-2310
(Phone) (301) 975-2008
(FAX) (301) 926-0416
(e-mail) data@nist.gov
(website) <http://www.nist.gov/srd>

If you have questions or problems pertaining to the use of the database, contact:

Piotr A. Domanski
National Institute of Standards and Technology
Engineering Laboratory
100 Bureau Drive, Stop 8631
Gaithersburg, MD 20899-8631
(e-mail) piotr.domanski@nist.gov

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