

**NIST**

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

Version 3.1

Users' Guide

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## CONTENTS

1. INTRODUCTION .....	1
2. INSTALLATION .....	3
3. MODELING OF LEAK AND RECHARGE PROCESS .....	4
4. DESCRIPTION OF THE PROGRAM .....	5
REFERENCES .....	7
Appendix A. SAMPLE RUN FOR LEAK PROCESS.....	8
Appendix B. SAMPLE RUN FOR LEAK AND RECHARGE PROCESS.....	16
Appendix C. ICONS .....	19
Appendix D. SINGLE-COMPONENT REFRIGERANTS AVAILABLE IN REFLEAK .....	20
Appendix E. PREDEFINED REFRIGERANT MIXTURES AVAILABLE IN REFLEAK .....	21
Appendix F. CONTACTS .....	22



## **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 the zeotropic mixtures, it may be important to predict the composition change under any of these leak conditions.

This REFLEAK program simulates leak and recharge processes for refrigerant zeotropic mixtures. This Windows-based program provides an easy-to-use package that allows estimation of composition changes of the zeotropic mixtures in leak and recharge processes for either vapor or liquid leaks under isothermal or adiabatic conditions. Studies related to the leak process of refrigerant mixtures were performed [1, 2]. Leak experiments of refrigerant mixtures have been compared with the simulation results [3, 4].

Thermodynamic properties of refrigerant mixtures are calculated based on the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 8.0 [5].

### **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 the temperature and 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 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.

### **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. Perhaps the property values obtained on either side of the error zone can be interpolated to satisfaction. It appears that the REFLEAK solution procedure taxes REFPROP property routines in unanticipated ways.

The program provides 'Help' sections to assist users. Several keywords are displayed in the help section, and users can choose a keyword by clicking on it.

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

Compared to the previous Version 2.1, this version of REFLEAK has incorporated the following changes:

1. REFPROP 8.0 property routines replaced REFPROP 7.0 routines.
2. The code of the program was modified to improve program's speed and convergence, including simulation cases with low initial volumetric quality.
3. The interface was changed to allow the user to view and modify the selection of the mixing rules and mixture parameters used by REFPROP property routines. This option is explained in Appendix A.

## **2. INSTALLATION**

### **System Requirements**

Free space for complete installation: 10.0 MB  
PC with Microsoft Windows 98/2000/Me/XP or NT 3.51/4.0

Printer: optional and should be Windows compatible  
Memory required: at least 32 MB

### **Installation Procedure**

In Windows NT 3.51, select File from the Program Manager's Menu Bar followed by Run from the File menu. In the entry box, type the CD-ROM drive letter and SETUP (e.g., D:SETUP) and press <enter>.

In Windows 98, NT 4.0, 2000, Me, XP click on the Start button and select Run. In the entry box, type the CD-ROM drive letter and SETUP (e.g., D:SETUP) and press <enter>.

Follow the remainder of the installation 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. In the leak process of a refrigerant mixture, 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 because the energy required for the vaporization is taken from the refrigerant remaining in the system and from the system wall.

Two idealized cases are considered in this program: isothermal and 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 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 system containers have a significant heat capacity, which will release some heat into the expanding vaporization process as the liquid temperature drops. Thus, an actual fast leak process probably falls 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 as the liquid during the liquid leak.

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. In modeling the recharge process, the liquid phase refrigerant in the charging cylinder is assumed to be put into the system. The mass of refrigerant recharged is the same as that leaked from the system. After recharging, the temperature in the system is "reset" to the initial temperature before the leak in the case of an adiabatic leak process.

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 properties of refrigerant mixtures in the simulation are calculated by the property routines included in the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 8.0 [5]. As a result, all limitations applicable to REFPROP (e.g., avoiding the critical point region) are equally applicable to REFLEAK.

#### **4. DESCRIPTION OF THE PROGRAM**

The leak/recharge simulation program 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 graphs.

When a user starts the program, the following actions can be taken step by step according to the user's need:

- (1) Choice of simulation mode: leak only or leak/recharge of a refrigerant mixture
- (2) Choice of leak situation: isothermal or adiabatic assumptions
- (3) Choice of leaking phase: vapor or liquid
- (4) Input of initial system temperature by typing number or by using the scroll bar
- (5) Input of initial volumetric quality by typing number or by using the scroll bar
- (6) Selection of refrigerant mixture for leak/recharge simulation

- a. Type in number of components
  - b. Selection of each mixture component from a list of possible refrigerants
  - c. Input of mass fraction of each component by typing numbers or by using the scroll bar
- or
- a. Click on the Predefined Mixture radio button
  - b. Select predefined mixture from list
- (7) Choose units for temperature, pressure, volume, and mass; (a) units for each may be individually selected or (b) all quantities may be reset to one of two choices corresponding to English or SI units
  - (8) Type in number of recharge cycles when simulating leak/recharge process
  - (9) Type in mass percentage loss for recharging the system

The main section for leak-only or leak/recharge simulation is comprised of one procedure, which is initiated by clicking on the 'Analyze' button. At this point, a new window for DOS opens to show intermediate stages of execution. All the data are used for plotting purposes. When the analysis is completed, this window disappears.

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

- (1) Displaying calculated results in a graphical format; the graph shows compositions of liquid and vapor phases as a function of leaked mass fraction. A vertical bar in the graph indicates specific values corresponding to x-axis value (leaked mass fraction). The data at this location is displayed in the lower part of the graph to show temperature, pressure, volumetric quality (void fraction), liquid specific volume, and vapor specific volume. Leaked mass fraction is displayed in the lower right corner of the screen. The limits of the y-axis can be changed via the Option button.
- (2) Saving output data in a file; the file name must be provided
- (3) Printing output data and/or graph

- (4) Redrawing a graph
- (5) Closing the display of data and graph

When a simulation for one refrigerant mixture is finished, the next simulation can be performed from the main window. A subsequent simulation can be carried out when a user selects conditions and repeats the several steps described in this section. If a user selects 'New' from 'File' menu, all the test conditions are set to the default values. In this case, the refrigerants should be selected separately again.

## REFERENCES

- [1] Kim, M.S. and Didion, D. A. , 1995, "Simulation of Isothermal and Adiabatic Leak Processes of Zeotropic Refrigerant Mixtures", Int. Journal of HVAC&R Research, ASHRAE, Atlanta, Georgia, USA, Vol. 1, No. 1, pp. 3-20.
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- [3] Shiflett, M.B., Yokozeki, A., and Reed, P.R., 1992, "Property and Performance Evaluation of 'SUVA' HP Refrigerants as R-502 Alternatives", Proc. of 1992 International Refrigeration Conference, Purdue Univ., West Lafayette, Indiana, U.S.A., Vol. 1, pp. 15-22.
- [4] Kruse, H. and Rinne, F., 1992, "Performance and Leakage Investigations of Refrigeration and Air-conditioning Systems Using Refrigerant Mixtures as Working Fluids", Proc. of 1992 International Refrigeration Conference, Purdue Univ., West Lafayette, Indiana, U.S.A., Vol. 2, pp. 621-630.
- [5] Lemmon, E. W., Huber, M. L., McLinden, M. O., 2007, NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 8.0. NIST Standard Reference Database 23, National Institute of Standards and Technology, Gaithersburg, Maryland, U.S.A.

## Appendix A

### SAMPLE RUN FOR LEAK PROCESS

A sample execution of the leak/recharge program to simulate the leak process is briefly described below. In this example, a leak process for a R32/134a mixture with a composition of 30/70 mass percentage is simulated. The leak process is assumed to be isothermal, and the vapor phase is leaking out of a system. Initial temperature is selected as 25 °C, and the initial volumetric quality, which is the ratio of the volume of vapor to the total volume, is selected as 0.2.

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

An introductory screen appears; click 'OK' to proceed.

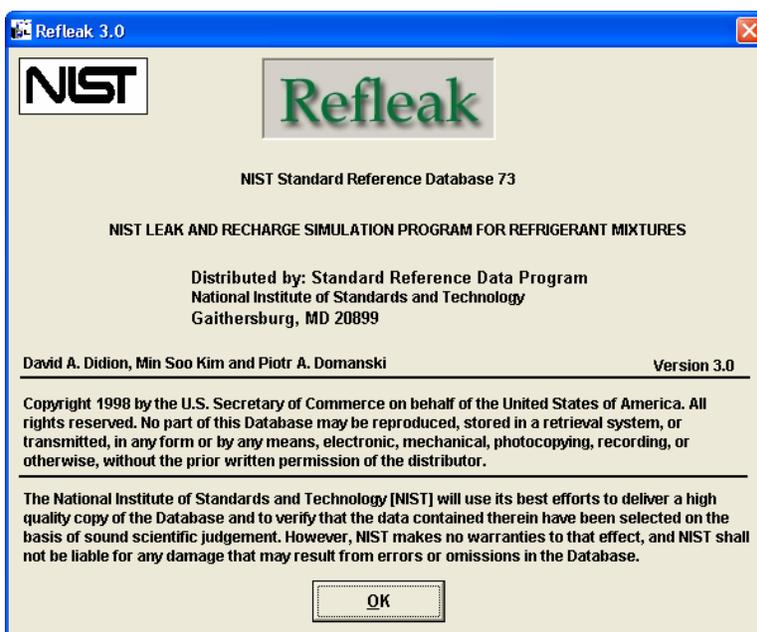


Figure A-1 Introductory screen of the program

The input screen is displayed next (Figure A-2). For this example, click 'Isothermal' in the leak process box and 'Vapor Phase' in the leaking phase box. Then, select an initial temperature (25.00) and initial volumetric quality (0.20) by typing in the numbers or by using the horizontal scroll bars. Click 'Leak Process Only' in the simulation box.

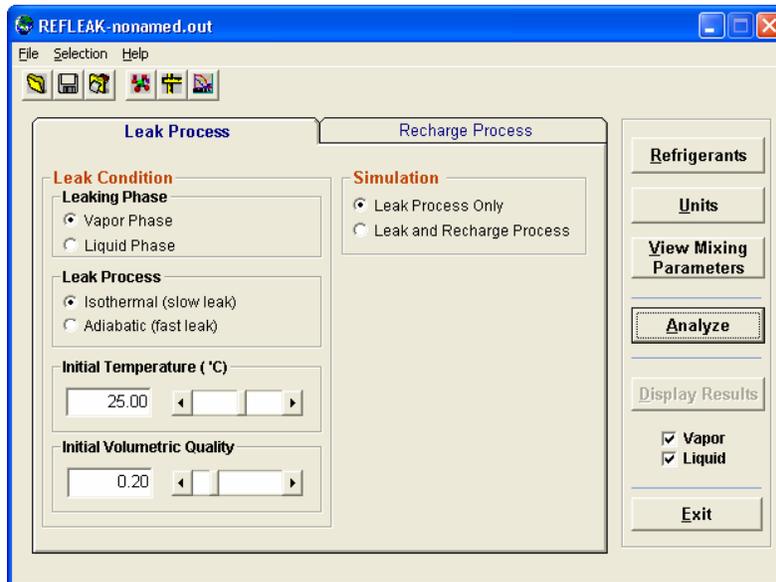


Figure A-2 Main window for data entry (leak process simulation)

Next, click on the button labeled 'Refrigerants' to specify the components. The screen shown in Figure A-3 is displayed. This input screen enables you to specify the mixture components desired.

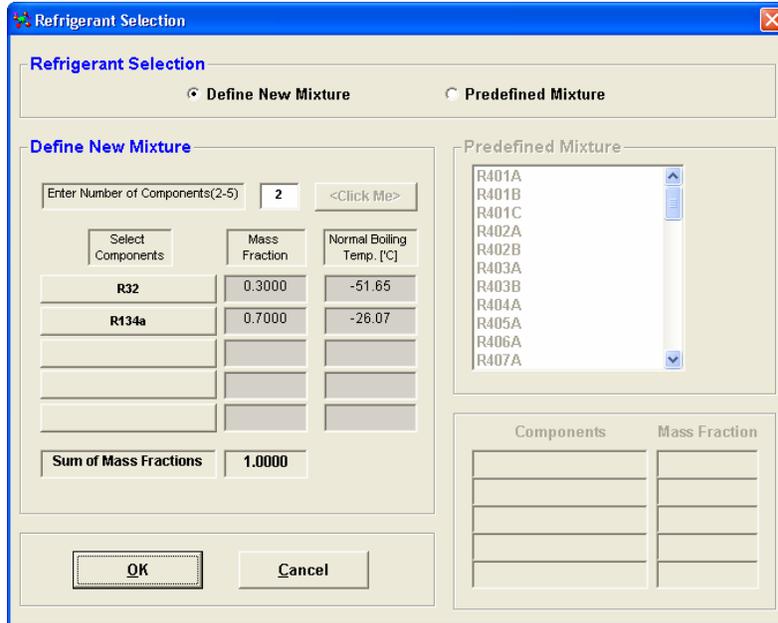


Figure A-3 Main window to determine refrigerants

Enter the number of components (here 2) in the box indicated and then click on the adjacent button. Next, click on the active 'Click Me' button in the left-hand column to select refrigerants. The window in Figure A-4 is then displayed.

An option for many of the mixtures that are commercially available is the predefined mixtures radio button. By clicking on the desired predefined mixture, the composition will appear in the lower right corner.

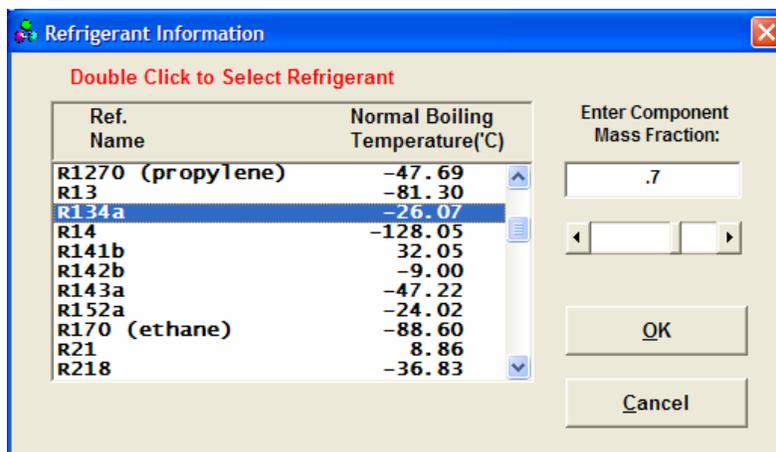


Figure A-4 Window for selection of refrigerant name and composition.

DOUBLE-CLICK (!) on the desired mixture component and enter the mass fraction in the upper right-hand box when prompted to do so. In this example, R32 with a mass fraction 0.30 and R134a with a mass fraction 0.70 have been selected. After selecting refrigerants and entering their respective mass fractions, click on the 'OK' button in the Refrigerant Selection window (Figure A-3).

From the main window for data entry (Figure A-2), you may enter the window "Mixing Parameters" (Figure A-5) to view and modify the selection of the mixing rule and mixture parameters used in calculating thermodynamic properties by the REFPROP routines. The window includes the short-hand name of the mixing rule, the numerical values for the parameters associated with that rule, and reference information. In a multi-component mixture, each binary pair may be edited. (When you click on the "Apply" button, a note "User defined" will be displayed for the particular refrigerant pair.

The mixing rule and values of mixing parameters displayed in the window – if they have not been altered by the user – are those recommended. Great care must be exercised in altering these choices. This option allowing the user to make changes in the

recommended mixing rules and mixing parameters is not intended for a casual user.

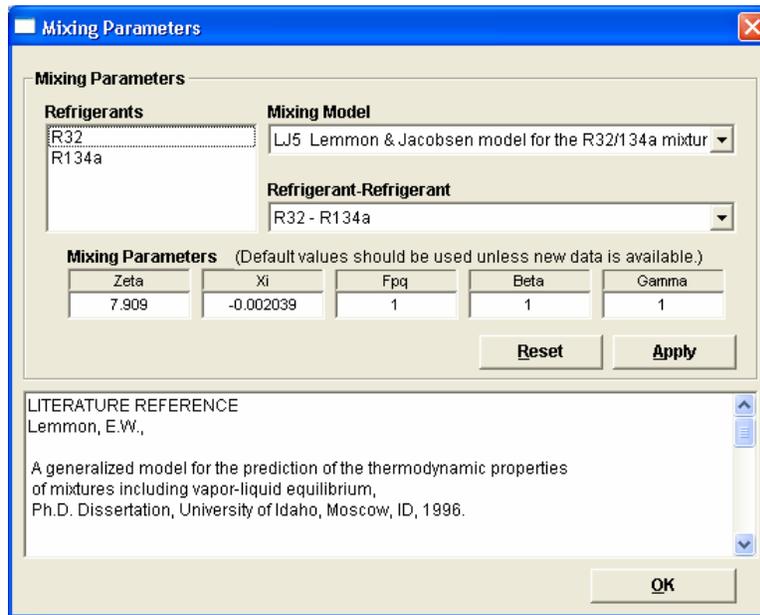


Figure A-5 Window for viewing and changing mixture parameters and mixing rules

If you wish to change units, click on the 'Units' button on the main window for data entry (Figure A-2). You can select any combination of the units individually for temperature, pressure, volume, and mass (Figure A-6). Consistent units can be selected by pressing 'SI' or 'English'.

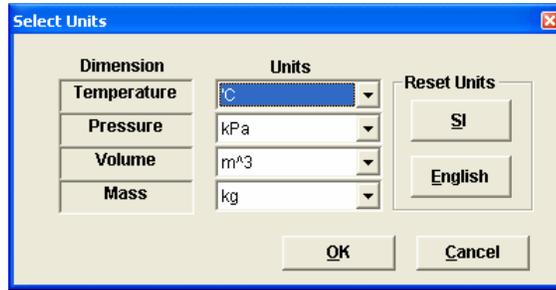


Figure A-6 Window for unit selection

Press 'Analyze' in the main window to start the simulation. (See Figure A-2).

During the execution, a DOS window appears to display the progress of simulation (Figure A-7). All the calculated data are used for printing or plotting purposes.

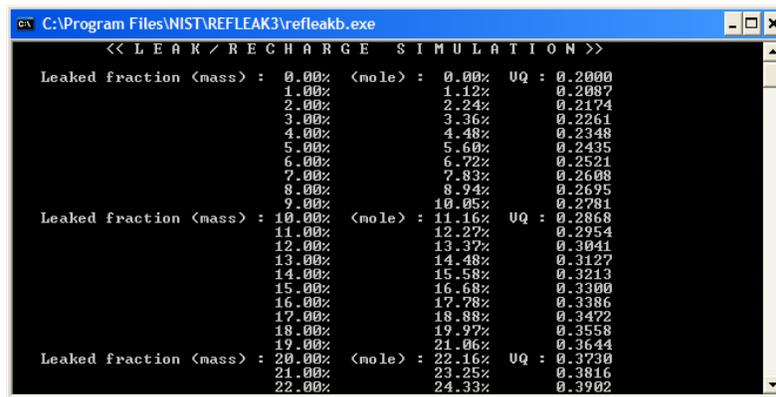


Figure A-7 Window to show the progress of a simulation (leak process)

When the calculations conclude, a graph (Figure A-8) is immediately 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 dragging it with the mouse, by typing x-axis values, or by scrolling a horizontal bar. At each mass percentage (x variable), vapor and liquid compositions including temperature, pressure, quality, liquid specific volume, and vapor specific volume are displayed.

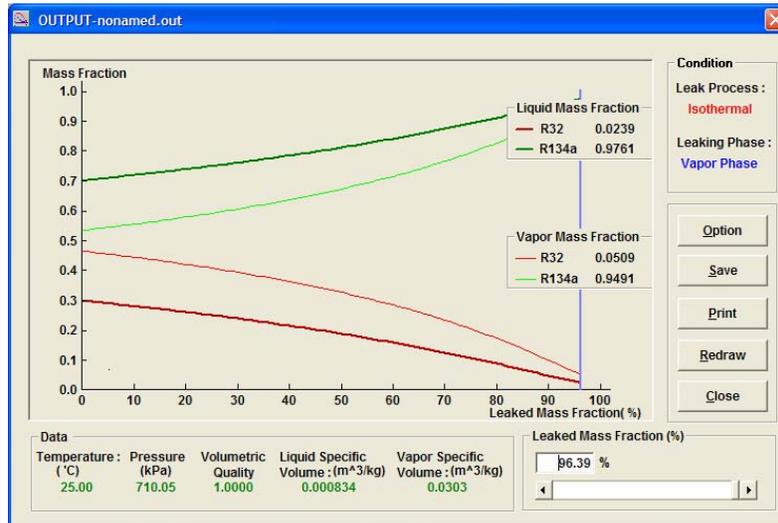


Figure A-8 Data display in a graph format (leak process)

To change the conditions for data display, click the 'Option' button to bring up the Output Option dialog (Figure A-9).

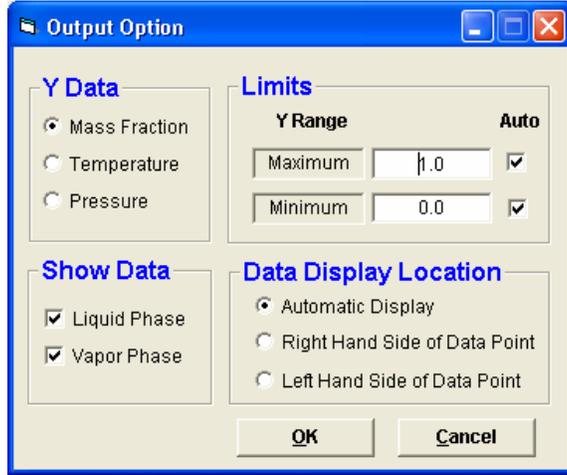


Figure A-9 Several options for data display

The data can be saved in a file by clicking on the 'Save' button. The data can be printed in tabular or graphical format by clicking the 'Print' button. When the 'Redraw' button is clicked, the graph is redrawn on the screen, during which time, the 'Redraw' button is replaced by 'Stop' or 'Continue' to toggle the redrawing process. Clicking on 'Close' returns to the main window.

## 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 a R32/134a mixture is simulated with initial composition of 30/70 percentage by mass. The leak process is assumed to be isothermal and the vapor phase is leaking out of a system. It is also assumed that the system is recharged when 30 % of the initial mass is leaked out of the system, and the system is recharged three times with the initial refrigerant composition. The temperature is 25 °C, and the initial volumetric quality (void fraction) is 0.2.

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

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

In the main window marked 'Leak Process', choose 'Isothermal' in the leak process box and 'Vapor Phase' in the leaking phase box. Select initial temperature (25.00) and initial volumetric quality (0.20) (see Figure A-2). Click 'Leak and Recharge Process' in the simulation box and the Recharge Process is displayed.

You can specify the number of recharge and mass percentage of loss for recharge by typing numbers or by using the scroll bars (see Figure B-1).

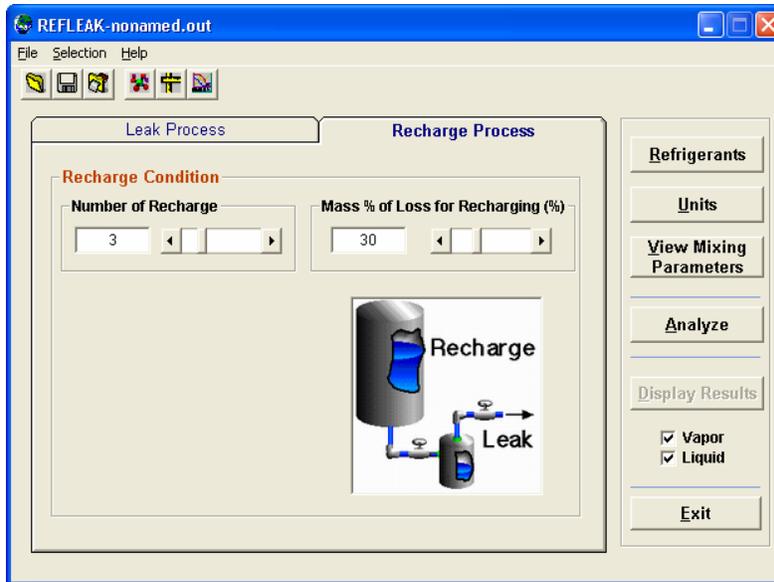


Figure B-1 Data entry window for leak and recharge simulation

Selection of a refrigerant mixture and units are the same as in Appendix A. (See Figure A-3, A-4, A-5)

Click on 'Analyze' to start the simulation.

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

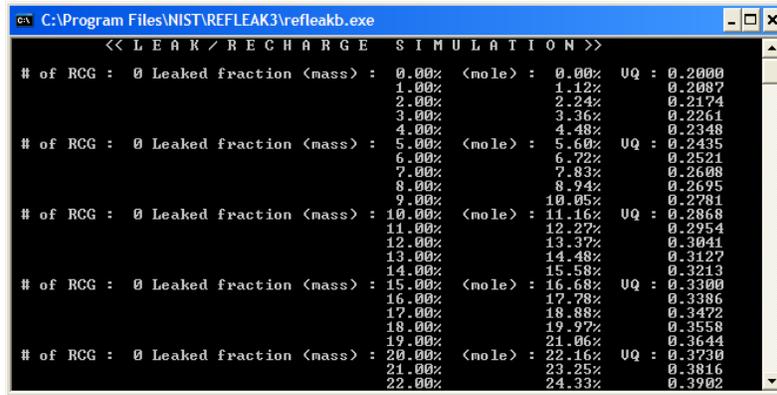


Figure B-2 Window to show a progress of simulation (leak and recharge process)

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

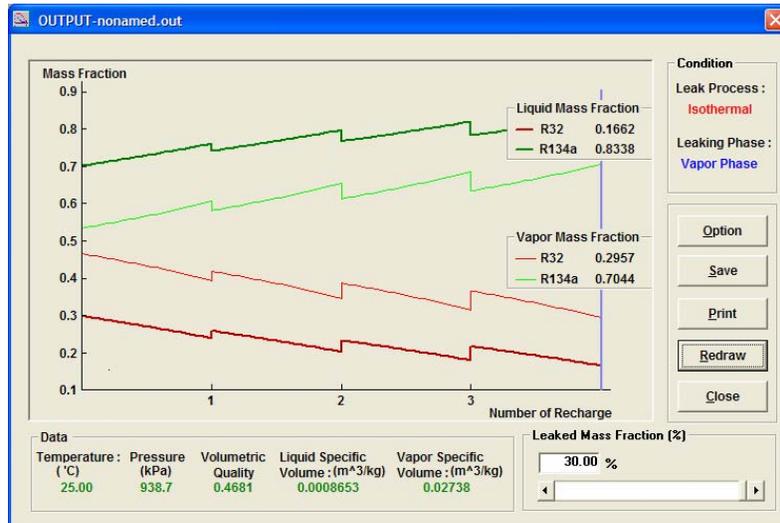


Figure B-3 Data display in graphical format (leak and recharge process)

## 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 <b>the file saved in a previous process</b>
	<u>S</u> ave	Save <b>the current process</b>
	<u>P</u> rint	Print <b>output</b>
	<u>R</u> efrigerant	Selection of refrigerants
	<u>O</u> utput	Display <b>output</b>
	<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		1,1-dichloro-2,2,2-trifluoroethane
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
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
R41		fluoromethane
R50		methane
R600		butane
R600a	or isobutane	2-methylpropane
R717		ammonia
R718		water

R740		argon
R744		carbon dioxide
RC318		octafluorocyclobutane
E170	or dimethylether	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
C3H6		propyne
C4H8	or trans-butene	trans-2-butene
CF3I		trifluoroiodomethane
C5F12	or perfluoropentane	dodecafluoropentane
SF6		sulfur hexafluoride

## 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/C318	45/7/5.5/42.5
R406A	R22/600a/142b	55/4/41
R407A	R32/125/134a	20/40/40
R407B	R32/125/134a	10/70/20
R407C	R32/125/134a	23/25/52
R407D	R32/125/134a	15/15/70
R407E	R32/125/134a	25/15/60
R408A	R125/143a/22	7/46/47
R409A	R22/124/142b	60/25/15
R409B	R22/124/142b	65/25/10
R410A	R32/125	50/50
R410B	R32/125	45/55
R411A	R1270/22/152a	1.5/87.5/11.0
R411B	R1270/22/152a	3/94/3
R412A	R22/218/142b	70/5/25
R413A	R218/143a/600a	9/88/3
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
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/R134a/R600/C5H12	5.1/93/1.3/0.6
R427A	R32/R125R143a/R134a	15/25/10/50
R428A	R125/R143a/R290/R600a	77.5/20/0.6/1.9
R500	R12/152a	73.8/26.2
R501	R22/12	75/25
R502	R22/115	48.8/51.2
R503	R23/13	40.1/59.9
R504	R32/115	48.2/51.8
R507A	R125/143a	50/50
R508A	R23/116	39/61
R508B	R23/116	46/54
R509A	R22/218	44/56

## Appendix F

### 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:

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

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