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

**Version 6.0
User's Guide**

J. Steven Brown
Piotr A. Domanski
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Young Jin Yoon

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1. INTRODUCTION

As alternatives to refrigerants with a high global warming potential (GWP), blends of two or more refrigerants are being utilized as working fluids in heat-pump, air-conditioning, and refrigeration systems, and in organic Rankine cycles. Generally, these blends form zeotropes, which show temperature and composition changes during evaporation, condensation, and flashing processes whether they are intended (i.e., through an expansion device) or unintended (e.g., a leak from a container or system). For zeotropic blends, it may be important and necessary to predict the composition change for any of these events.

REFLEAK simulates leak and recharge processes for zeotropic refrigerant blends. This Windows-based simulation model provides an easy-to-use package that allows estimation of composition changes of zeotropic blends in leak and recharge processes for either vapor or liquid leaks under isothermal or adiabatic conditions. The generic model of these processes used in REFLEAK and example simulation studies are presented in [1, 2]. Other computer simulations and laboratory leak measurements of specific blends are reported in [3, 4].

Thermodynamic properties of the refrigerant blends are calculated using the NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties – REFPROP, Version 10.0 [5].

Uncertainties in Calculated Properties

The objective in selecting fluid 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 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 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 blends, which 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 meet the user's needs.

The simulation model provides 'Help' sections with several keywords to assist the user.

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

Compared to version 4.0, version 5.0 of REFLEAK included a Graphical User Interface (GUI) built on the .NET platform of Microsoft® and extended to 10 the number of refrigerants allowed in a blend. This version 6.0 migrates REFLEAK from REFPROP 9.1 to REFPROP 10.0 for the representation of thermophysical properties. This transition expands the list of refrigerants to those available in REFPROP 10.0, including new low-GWP fluids (Appendix D).

2. INSTALLATION

System Requirements

- Personal computer capable of running Microsoft Windows 7, 8, 10 with Microsoft .NET Framework version 4.7.2 or later and Microsoft Visual C++ Runtime Library (for x86) version 14 or later.
- A hard disk with 17 megabytes of available space. The installation process will require additional 104 MB of space for Microsoft .NET Framework version 4.7.2 and Microsoft Visual C++ Runtime Library (for x86) version 14 if they are not installed already.
- The screen resolution should be set to 1024 x 768 or higher to view images in their entirety.

Installation Procedure

Execute the REFLEAK installation file setup.exe with REFLEAK 6.0 Installer.msi residing in the same directory. Follow the on-screen instructions. To run the program, click on the REFLEAK icon on the Start Menu.

3. MODELING OF LEAK AND RECHARGE PROCESS

During a leak process of a refrigerant zeotropic blend, 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 removed from the refrigerant remaining in the system and from the system material.

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 remains constant because of the heat transfer through the walls from the environment. In an 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 blend 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 a vapor leak, and the same composition as the liquid during a 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. 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 using the property routines included in the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 10.0 [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 sections: (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 and/or print graphs.

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

- (1) Select the refrigerant blend for the leak/recharge simulation. Note that the refrigerant blend must be chosen before any other data can be input or action taken, except that of changing units.
 - a. For a predefined blend, press the appropriately labeled command button.
 - b. For a user-defined blend, press the appropriately labeled command button.
 - i. Select up to ten components from the list box.
 - 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) Choose the simulation mode: leak only or leak/recharge.
- (3) Choose the type of leak: isothermal or adiabatic.
- (4) Choose the leaking phase: vapor or liquid.
- (5) Choose SI or IP (Inch-Pound) units.
- (6) Input the initial leak condition by specifying:
 - a. Initial refrigerant temperature.
 - b. Initial vapor volumetric quality.

Optionally, the initial vapor volumetric quality at the leak 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 of this report outlines the calculation procedure used by REFLEAK. Note that 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) Input the number of recharge cycles when simulating the leak/recharge process.
- (8) Input 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 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) Display of the calculated results in graphical format (Figures A-14 and B-2); the graph shows mass compositions of the liquid and vapor phases as a function of the leaked mass. A vertical blue line in the graph indicates the specific location on the x-axis (leaked mass (%)) for which mass compositions are displayed. The location of the vertical bar can be changed to a specific value of the leaked mass (%) via the slider bar located in the lower right corner of the screen. Data at this specific value of leaked mass 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 change the limits of the y-axis by using the 'y-Axis Limits' frame.
- (3) Print the graph with data.
- (4) Redraw the graph.
- (5) Save numerical simulation results.
- (5) Close the display of data and graph.

The input data can be stored to a file using the 'Save' or 'Save as' command from the File menu. The file with data is saved to C:\Users\ xxx\Documents\REFLEAK data, where 'xxx' is the user name on a given computer, unless the user selects a different location.

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 blend 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 that if the user modifies any of the data after a simulation has been run, the previous simulation results will be removed from memory.

REFERENCES

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- [6] American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc., (ASHRAE), 2016. ANSI/ASHRAE Standard 34-2016, Designation and Safety Classification of Refrigerants.
- [7] McLinden, M.O., 2007, Private communication.

Appendix A

EXAMPLE RUN FOR LEAK PROCESS

A sample execution of the leak/recharge simulation model for a leak process is 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 0.30.

To start the simulation model double click the REFLEAK icon. An introductory screen appears.

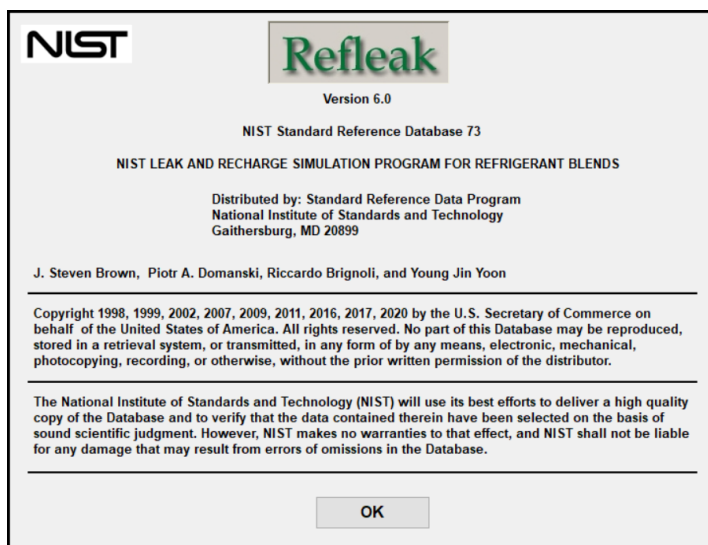


Figure A-1. Introductory screen

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.

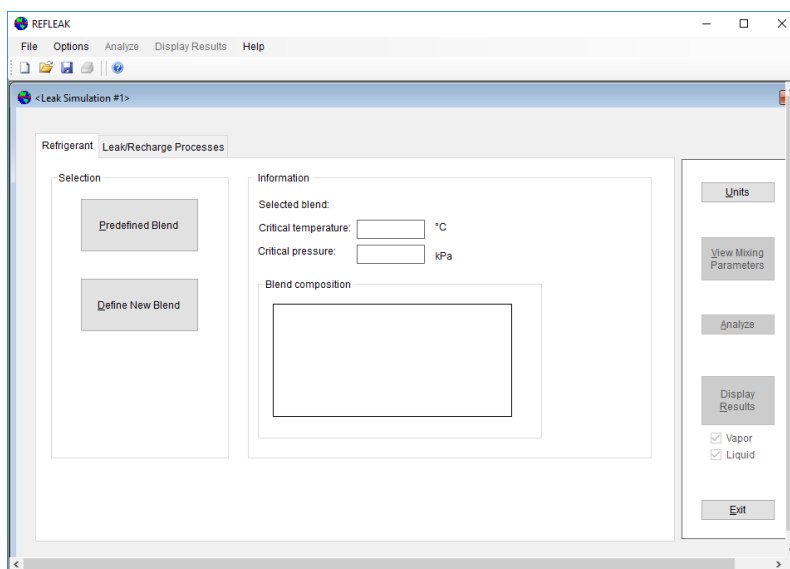


Figure A-2. Main window for data entry

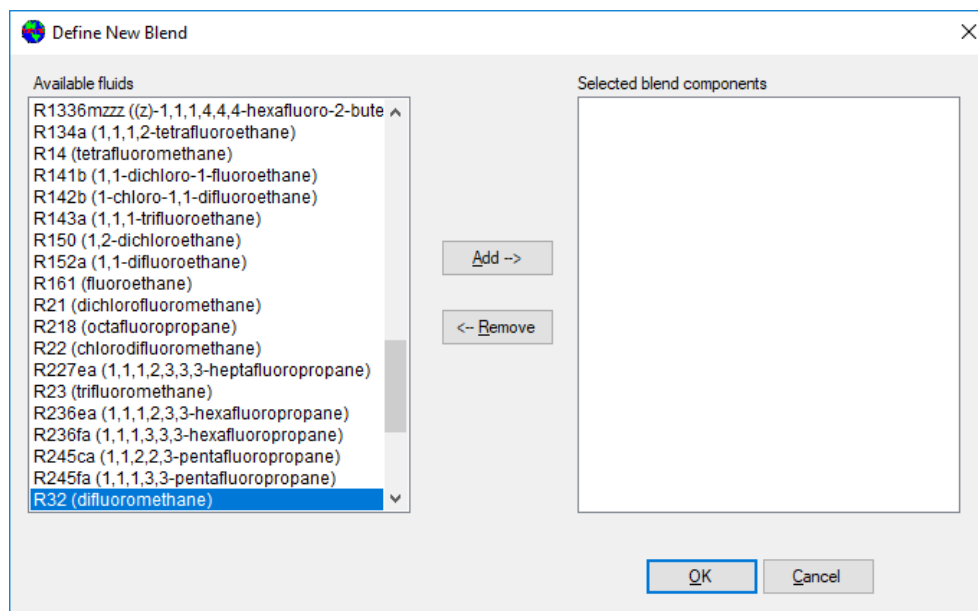


Figure A-3. Window for selecting components for a user-defined blend

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 blend, 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.

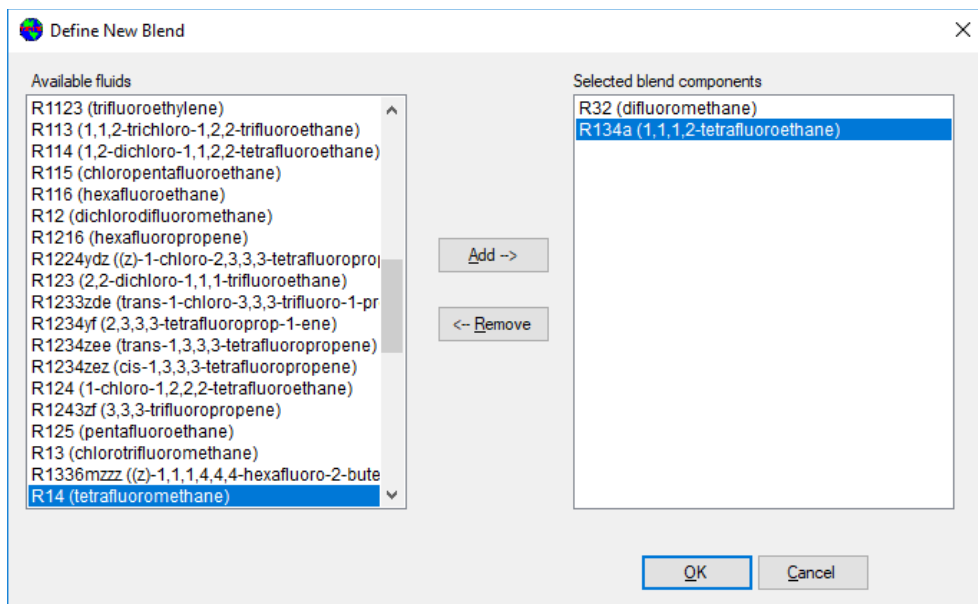


Figure A-4. Appearance of window after selection of refrigerants

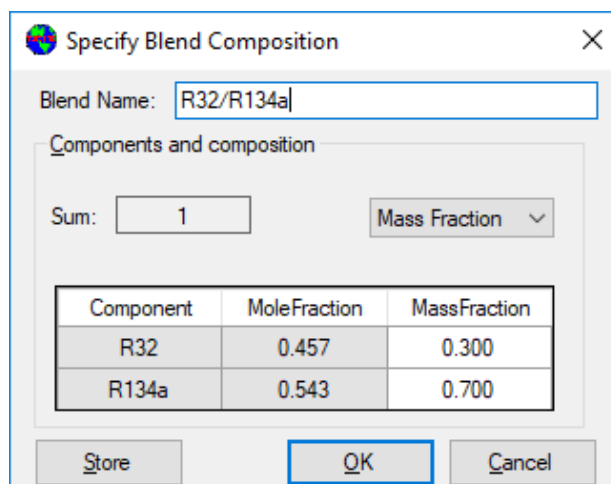


Figure A-5. Window for specifying blend composition

The specified blend can be stored as a predefined blend by clicking the command button 'Store', after which Figure A-6 will appear. To proceed with the 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'.

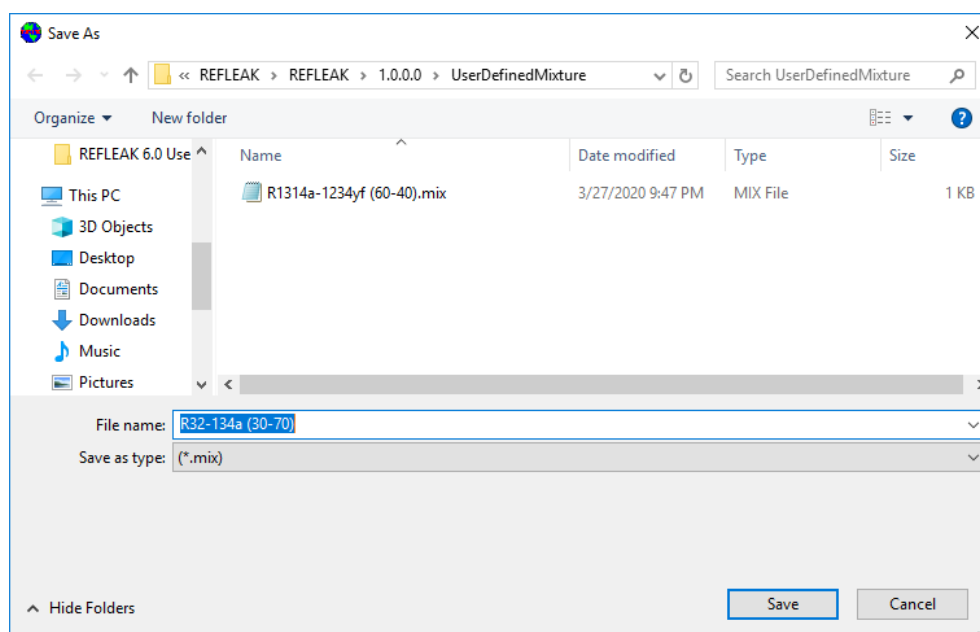


Figure A-6. Storing the user-defined blend for later use as a predefined blend

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 enabled. Also, the checkboxes 'Vapor' and 'Liquid' are enabled. By alternately clicking one or both of the checkboxes 'Vapor' and/or 'Liquid,' 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.

REFLEAK

File Options Analyze Display Results Help

<Leak Simulation #1>

R32-134a (30-70)

Refrigerant Leak/Recharge Processes

Selection

Predefined Blend

Define New Blend

Information

Selected blend: R32-134a (30-70)

Critical temperature: 91.57 °C

Critical pressure: 4858.16 kPa

Blend composition

Component	Mole Fraction	Mass Fraction
R32	0.457	0.300
R134a	0.543	0.700

Units

View Mixing Parameters

Analyze

Display Results

☒ Vapor

☒ Liquid

Exit

Figure A-7. Main data entry window after specification of blend

REFLEAK

File Options Analyze Display Results Help

<Leak Simulation #1>

R32-134a (30-70)

Refrigerant Leak/Recharge Processes

Leak Type

☒ Isothermal (slow leak)

☐ Adiabatic (fast leak)

Leaking Phase

☒ Vapor Phase

☐ Liquid Phase

Simulations

☒ Leak Process Only

☐ Leak and Recharge Process

Recharge Process

Number of Recharges

Percent mass loss for recharging

Initial Leak Condition

Initial Temperature: 25.00 °C

Initial Volumetric Quality: 0.300 mol/mol

Optional Calculation of Initial Volumetric Quality

Fill Temperature: °C

Fraction of Maximum Liquid Fill:

Calculate

Units

View Mixing Parameters

Analyze

Display Results

☒ Vapor

☒ Liquid

Exit

Figure A-8. Main data entry window with default selections for leak/recharge Processes

The default values are 25.0 °C for the initial temperature and 0.2 for the initial vapor 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 radio button, or modify the desired value in the appropriate data boxes. To continue with this example, place the cursor in the 'Initial Volumetric Quality'

data box, and enter the value 0.30. If one were to err while typing the input data, a message such as the one shown in Figure A-9 will appear.

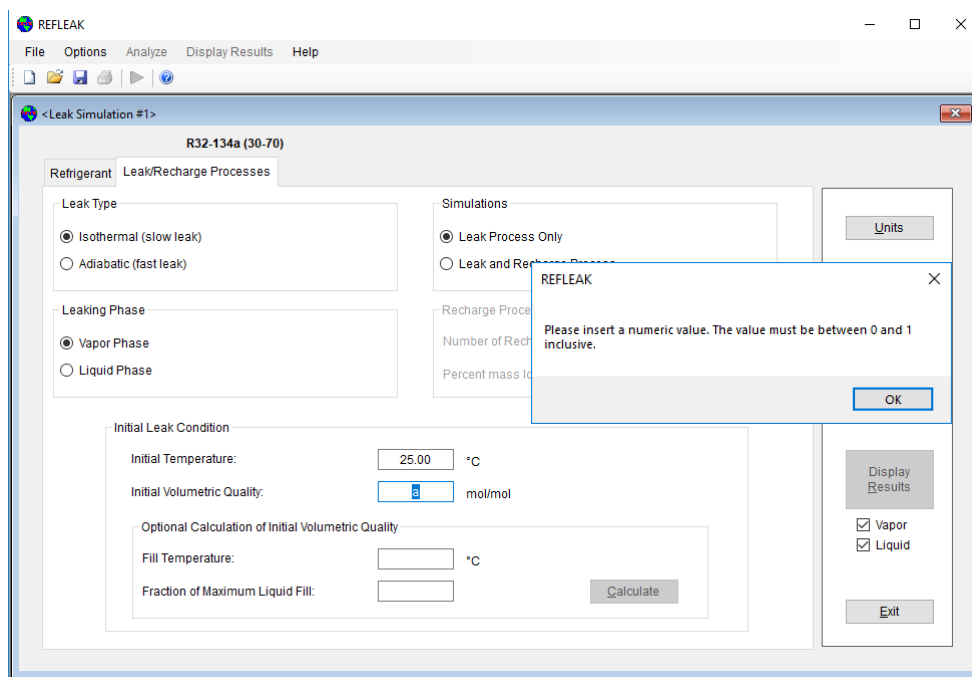


Figure A-9. Sample error message resulting from the mistyping of input data

Alternately, to implement the optional calculation procedure for initial volumetric quality, click either the 'Fill Temperature' data box or the 'Fraction of Max. Liquid Fill' data box and enter the values, which will enable the 'Calculate' command button (Figure A-10). For this example, the fill temperature was 54.4 °C, and the value for fraction of maximum liquid fill that results in the initial volumetric quality of 0.30 is entered. Once the command button 'Calculate' has been clicked, the window shown in Figure A-11 will appear. Now, the 'Analyze' command button is enabled. To once again specify the initial volumetric quality, 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.

The screenshot shows the REFLEAK software interface. The main window is titled "<Leak Simulation #1>" and displays the "R32-134a (30-70)" refrigerant. The "Leak/Recharge Processes" tab is active. Under "Leak Type", "Isothermal (slow leak)" is selected. Under "Leaking Phase", "Vapor Phase" is selected. In the "Initial Leak Condition" section, "Initial Temperature" is 25.00 °C, "Initial Volumetric Quality" is empty, "Fill Temperature" is 54.40 °C, and "Fraction of Maximum Liquid Fill" is 0.808. The "Optional Calculation of Initial Volumetric Quality" section is visible. On the right, there are buttons for "Units", "View Mixing Parameters", "Analyze", "Display Results", and "Exit". The "Display Results" button has checkboxes for "Vapor" and "Liquid", both of which are checked.

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

The screenshot shows the REFLEAK software interface after the "Calculate" button has been clicked. The "Initial Leak Condition" section now shows "Initial Volumetric Quality" as 0.300 mol/mol. The "Optional Calculation of Initial Volumetric Quality" section is still visible, but the "Calculate" button is now disabled. The rest of the interface, including the "Leak Type", "Leaking Phase", and "Simulations" sections, remains the same as in Figure A-10.

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 blend 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 blend model is based on pairs of components. For multicomponent blends, each binary pair is viewed separately.

Note that changing the mixing rules and mixing parameters is **not intended** for a non-expert 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.

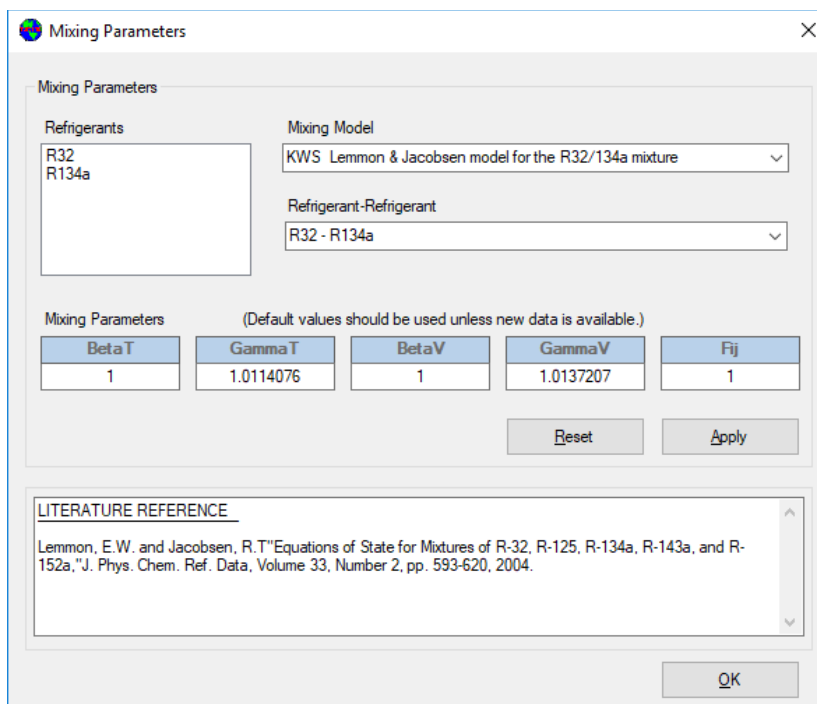


Figure A-12. Window for viewing and changing blend mixing models and parameters

To change the units, click the command button 'Units' on the main window for data entry (Figure A-2), after which Figure A-13 will appear.

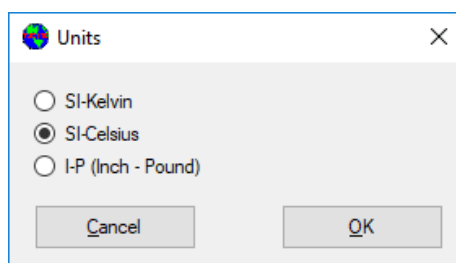


Figure A-13. Selection of units

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

After the simulation is completed, a graph (Figure A-14) 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 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.

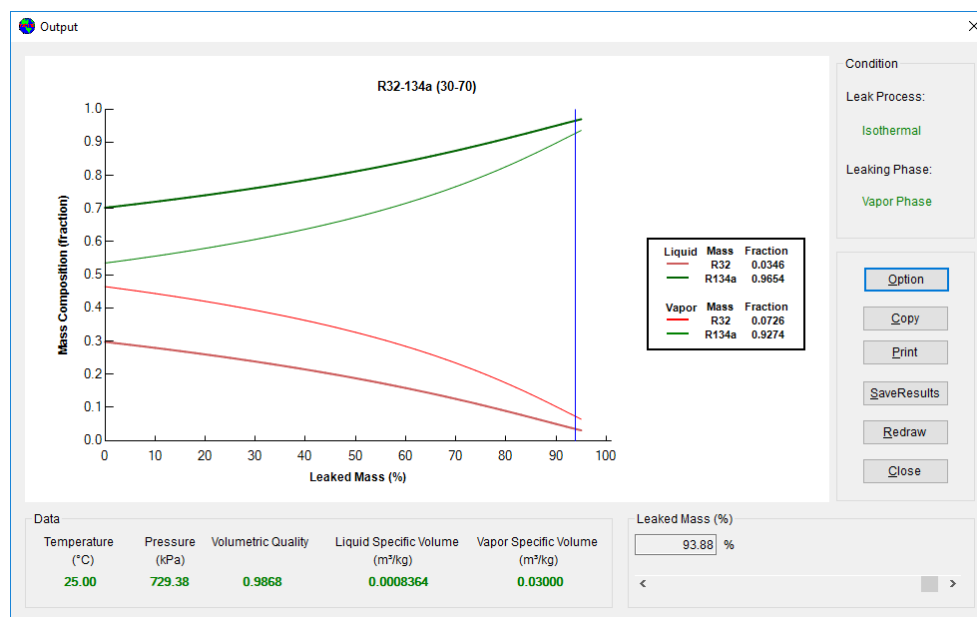


Figure A-14. Data display in a graph format (leak process)

To change the options for data display, click the command button 'Option', after which the window shown in Figure A-15 will appear.

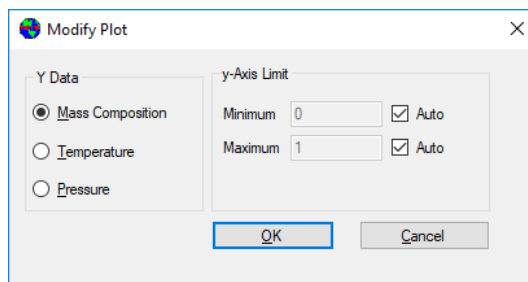



Figure A-15. Options for data display

The data can be printed in graphical format by clicking the command button 'Print', selecting the menu item 'File/Print', or clicking the toolbar icon . The numerical results can be saved in a comma-separated values (CSV) file by clicking the 'SaveResults' button.

When the command button 'Redraw' is clicked, the graph is redrawn on the screen.

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

Appendix B

EXAMPLE RUN FOR LEAK AND RECHARGE PROCESS

This section describes an example of a leak and recharge process for the R134a/1234yf blend simulated with the initial composition of 60/40 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. Each time, the initial leak temperature is 20 °C, and the initial volumetric quality is 0.20.

Double click the REFLEAK icon.

An introductory screen appears (See Figure A-1).

Follow the steps shown in Appendix A to select the refrigerant. Click the tab 'Leak/Recharge Processes' following the steps in Appendix A. Click the radio button 'Leak and Recharge Process'. Input 3 into the 'Number of recharges' data box and input 30 in the 'Percent mass loss for recharging' data box, as shown in Figure B-1.

In the next step enter the initial leak temperature to be 20 °C and the initial volumetric quality to be 0.20.

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. After the simulation, the output is displayed in graphical format as shown in Figure B-2.

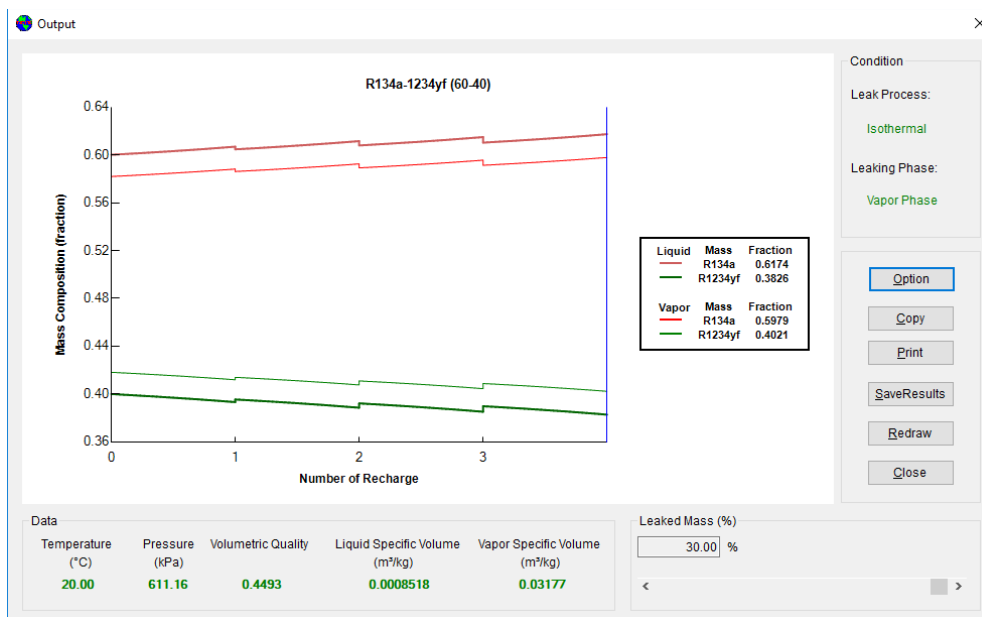



Figure B-2. Data display in graphical format (leak and recharge process)

The user can reproduce this run using the example file R134a-1234yf (60-40) leak-recharge.xml. This file can be loaded by selecting the menu item 'File/Open' or by clicking the toolbar icon  and selecting the "Examples" folder (Figure B-3).

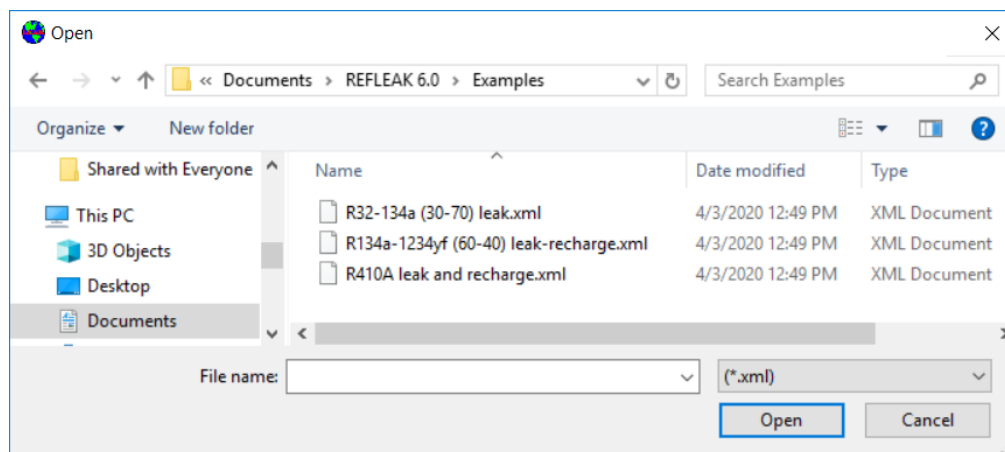








Figure B-3. Example run files

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>N</u> ew	Begin a new analysis
	<u>O</u> pen	Open previous analysis
	<u>S</u> ave	Save the analysis
	<u>P</u> rint	Print results
	<u>A</u> nalyze	Run simulation
	<u>H</u> elp	Open help file

Appendix D

SINGLE-COMPOUND FLUIDS AVAILABLE IN REFLEAK

Short Name	Full Chemical Name	T_{crit} (°C)	T_{crit} (°F)
R-11	trichlorofluoromethane	198.0	388.3
R-12	dichlorodifluoromethane	112.0	233.6
R-13	chlorotrifluoromethane	29.2	84.6
R-1311	trifluoroiodomethane	123.3	253.9
R-14	tetrafluoromethane	-45.6	-50.2
R-21	dichlorofluoromethane	178.3	353.0
R-22	chlorodifluoromethane	96.2	205.1
R-23	trifluoromethane	25.9	78.7
R-32	difluoromethane	78.1	172.6
R-40	methyl chloride	143.2	289.7
R-41	fluoromethane	44.1	111.4
R-50	methane	-116.7	-82.7
R-113	1,1,2-trichloro-1,2,2-trifluoroethane	214.1	417.3
R-114	1,2-dichloro-1,1,2,2-tetrafluoroethane	145.7	294.2
R-115	chloropentafluoroethane	80.0	175.9
R-116	hexafluoroethane	19.9	67.8
R-123	1,1-dichloro-2,2,2-trifluoroethane	183.7	362.6
R-124	1-chloro-1,2,2,2-tetrafluoroethane	122.3	252.1
R-125	pentafluoroethane	66.2	151.1
R-134a	1,1,1,2-tetrafluoroethane	101.1	213.9
R-141b	1,1-dichloro-1-fluoroethane	204.2	399.6
R-142b	1-chloro-1,1-difluoroethane	137.1	278.8
R-143a	1,1,1-trifluoroethane	72.9	163.2
R-152a	1,1-difluoroethane	113.3	235.9
R-161	fluoroethane	102.2	215.9
R-170	ethane	32.2	89.9
R-218	octafluoropropane	161.5	72.0
R-227ea	1,1,1,2,3,3,3-heptafluoropropane	102.8	217.0
R-236ea	1,1,1,2,3,3-hexafluoropropane	139.3	282.7
R-236fa	1,1,1,3,3,3-hexafluoropropane	124.9	256.9
R-245ca	1,1,2,2,3-pentafluoropropane	174.4	346.0
R-245fa	1,1,1,3,3-pentafluoropropane	154.1	309.3
R-365mfc	1,1,1,3,3-pentafluorobutane	186.9	368.3
R-290	propane	96.7	206.1
R-C318	octafluorocyclobutane	115.2	239.4
R-600	butane	152.0	305.6
R-600a	isobutane or 2-methylpropane	134.7	274.5
R-717	ammonia	132.3	270.1
R-744	carbon dioxide	31.1	87.9
R-1150	ethylene	9.2	48.6
R-1216	hexafluoropropene	85.8	186.4
R-1233zd(E)	1-chloro-3,3,3-trifluoroprop-1-ene	166.5	330.1
R-1234yf	2,3,3,3-tetrafluoroprop-1-ene	94.7	202.5
R-1234ze(E)	trans-1,3,3,3-tetrafluoropropene	109.4	228.9
R-1234ze(Z)	cis-1,3,3,3-tetrafluoropropene	150.1	302.2
R-1243zf	3,3,3-trifluoropropene	103.8	218.8
R-1270	propylene or propene	92.4	198.4
RE-143a	methyl-trifluoromethyl-ether	104.8	220.6
RE-170	dimethylether or ethylene oxide	127.2	260.9

Short Name	Full Chemical Name	T_{crit} (°C)	T_{crit} (°F)
RE-245cb2	methyl-pentafluoroethyl-ether	133.7	272.6
RE-245fa2	2,2,2-trifluoroethyl-difluoromethyl-ether	171.7	341.1
RE-347mcc	1,1,1,2,2,3,3-Heptafluoro-3-methoxypropane	164.6	328.2
CH ₃ CH ₂ CH=CH ₂	1-butene	146.1	295.1
Cyclo-C ₃ H ₆	cyclopropane	125.2	257.3
C ₂ H ₆ O	ethanol or ethyl alcohol	240.8	465.4
CH(CH ₃) ₃	isobutene or 2-methyl-1-propene	144.9	292.9
(CH ₃) ₂ CH(CH ₂) ₂ CH ₃	isohexane or 2-methylpentane	224.6	436.2
(CH ₃) ₂ CHCH ₂ CH ₃	isopentane or 2-methylbutane	187.2	369.0
CH ₃ OH	methanol	239.5	463.0
CH ₃ -3(CH ₂)-CH ₃	pentane	196.6	385.8
C ₃ H ₆ O	acetone	235.0	454.9
C ₄ H ₈	cis-butene or cis-2-butene	162.6	324.7
C ₄ H ₈	trans-butene or trans-2-butene	155.5	311.8
C ₅ F ₁₂	perfluoropentane or dodecafluoropentane	147.4	297.3
C ₅ H ₁₂	neopentane or 2,2-dimethylpropane	160.6	321.1
C ₆ H ₆	benzene	288.9	552.0
C ₆ H ₁₂	cyclohexane	280.5	536.9
C ₆ H ₁₄	hexane	234.7	454.4
C ₇ H ₁₆	heptane	267.0	512.6
C ₁₂ H ₂₆	dodecane	385.0	724.9
SF ₆	sulfur hexafluoride	45.6	114.0

The user can add a new fluid to REFLEAK by placing a new fluid file into two 'fluids' folders. The fluid file must be compatible with REFPROP 10.0, and its name must start with "R" or "r" (e.g., Rnew2.fld or r754.fld will be recognized by REFLEAK as fluid files).

The two 'fluids' folders containing REFPROP fluid files are located at the following locations:

- REFLEAK main folder in which the REFLEAK.exe has been installed. The default locations is:
C:\Program Files (x86)\NIST\REFLEAK 6.0\FLUIDS
- C:\Users\xxx\AppData\Local\REFLEAK\REFLEAK 6.0\1.0.0.0\FLUIDS

where 'xxx' is the user name on a given computer. This path may be hidden according to the Windows setting. To get the path visible, on 'Windows Search' type 'Folder Options', open the 'Folder Options' window, select the 'View' tab; under 'Hidden files and folders' check 'Show hidden files, folders and drives'.

Appendix E

PREDEFINED REFRIGERANT BLENDS AVAILABLE IN REFLEAK

ASHRAE Designation	Components	Composition (mass %)	T_{crit} (°C)	T_{crit} (°F)
R-401A	R-22/152a/124	53/13/34	106.9	224.3
R-401B	R-22/152a/124	61/11/28	104.6	220.3
R-401C	R-22/152a/124	33/15/52	111.7	233.1
R-402A	R-125/290/22	60/2/38	74.8	166.6
R-402B	R-125/290/22	38/2/60	82.1	179.7
R-403A	R-290/22/218	5/75/20	84.0	183.2
R-403B	R-290/22/218	5/56/39	75.4	167.8
R-404A	R-125/143a/134a	44/52/4	72.1	161.8
R-405A	R-22/152a/142b/C318	45/7/5.5/42.5	104.3	219.8
R-406A	R-22/600a/142b	55/4/41	115.5	239.8
R-407A	R-32/125/134a	20/40/40	82.3	180.1
R-407B	R-32/125/134a	10/70/20	74.8	166.6
R-407C	R-32/125/134a	23/25/52	86.1	187.1
R-407D	R-32/125/134a	15/15/70	91.6	196.9
R-407E	R-32/125/134a	25/15/60	88.6	191.5
R-407F	R-32/125/134a	30/30/40	82.6	180.7
R-407G	R-32/125/134a	2.5/2.5/95	99.5	211.0
R-408A	R-125/143a/22	7/46/47	82.9	181.3
R-409A	R-22/124/142b	60/25/15	110.1	230.1
R-409B	R-22/124/142b	65/25/10	107.6	225.7
R-410A	R-32/125	50/50	71.3	160.4
R-410B	R-32/125	45/55	70.8	159.5
R-411A	R-1270/22/152a	1.5/87.5/11.0	88.9	191.9
R-411B	R-1270/22/152a	3/94/3	95.7	204.2
R-412A	R-22/218/142b	70/5/25	107.1	224.8
R-413A	R-218/143a/600a	9/88/3	95.3	203.6
R-414A	R-22/124/600a/142b	51/28.5/16.5	111.4	232.5
R-414B	R-22/124/600a/142b	50/39/1.5/9.5	110.7	231.3
R-415A	R-22/152a	82/18	96.7	206.0
R-415B	R-22/152a	25/75	109.9	229.9
R-416A	R-124/R134a/600	39.5/59.0/1.5	106.3	223.3
R-417A	R-125/134a/600	46.6/50.0/3.4	85.4	185.8
R-417B	R-125/134a/600	79.0/18.3/2.7	74.1	165.3
R-417C	R-125/134a/600	19.5/78.8/1.7	94.6	202.2
R-418A	R-290/22/152a	1.5/96/2.5	95.6	204.2
R-419A	R-125/134a/DME	77/19/4	83.5	182.3
R-419B	R-125/134a/DME	48.5/48/3.5	91.1	196.0
R-420A	R-134a/142b	88/12	104.8	220.6
R-421A	R-125/134a	58/42	82.8	181.0
R-421B	R-125/134a	85/15	72.4	162.3
R-422A	R-125/134a/600a	85.1/11.5/3.4	70.7	159.3
R-422B	R-125/134a/600a	55/42/3	82.0	179.6
R-422C	R-125/134a/600a	82/15/3	72.1	161.7
R-422D	R-125/134a/600a	65.1/31.5/3.4	78.2	172.8
R-422E	R-125/134a/600a	58/39.3/2.7	81.1	178.0
R-423A	R-134a/227ea	52.5/47.5	99.1	210.5
R-424A	R-125/134a/600a/600/601a	50.5/47/0.9/1/0.6	84.7	184.4
R-425A	R-32/134a/227ea	18.5/69.5/12	93.9	210.4
R-426A	R-125/134a/600/601a	5.1/93/1.3/0.6	99.0	210.2
R-427A	R-32/125/143a/134a	15/25/10/50	85.5	185.9

ASHRAE Designation	Components	Composition (mass %)	T_{crit} (°C)	T_{crit} (°F)
R-428A	R-125/143a/290/600a	77.5/20/0.6/1.9	68.0	154.4
R-429A	DME/152a/600a	60/10/30	122.0	251.5
R-430A	R-152a/600a	6/24	107.0	224.6
R-431A	R-290/152a	71/29	91.8	197.2
R-432A	R-1270/DME	80/20	97.3	207.1
R-433A	R-1270/290	30/70	94.4	201.9
R-433B	R-1270/290	5/95	96.3	205.4
R-433C	R-1270/290	25/75	94.8	202.6
R-434A	R-125/143a/134a/600a	63.2/18/16/2.8	74.1	165.5
R-435A	DME/152a	80/20	123.1	253.5
R-436A	R-290/600a	56/44	115.9	240.6
R-436B	R-290/600a	52/48	117.4	243.4
R-437A	R-125/134a/600/601a	19.5/78.5/1.4/0.6	95.5	203.9
R-438A	R-32/125/134a/600/601a	8.5/45/44.2/1.7/0.6	83.8	182.9
R-439A	R-32/125/600a	50/47/3	70.3	158.6
R-440A	R-290/134a/152a	0.6/1.6/97.8	112.7	234.8
R-441A	R-170/290/600a/600	3/55/6/36	118.5	245.2
R-442A	R-32/125/134a/152a/227ea	31/31/30/3/5	82.1	179.9
R-443A	R-1270/290/600a	55/40/5	96.0	204.8
R-444A	R-32/152a/1234ze(E)	12/5/83	106.3	223.4
R-444B	R-32/152a/1234ze(E)	41.5/10/48.5	95.7	204.2
R-445A	R-744/134a/1234ze(E)	6/9/85	106.1	222.9
R-446A	R-32/1234ze(E)/600	68/29/3	86.1	186.9
R-447A	R-32/125/1234ze(E)	68/3.5/28.5	85.3	185.5
R-448A	R-32/125/1234yf/134a/1234ze(E)	26/26/20/21/7	82.7	180.8
R-449A	R-32/125/1234yf/134a	24.3/24.7/25.3/25.7	82.1	179.7
R-449B	R-32/125/1234yf/134a	25/24/23/27	82.2	180.0
R-450A	R-134a/1234ze(E)	42/58	104.5	220.0
R-451A	R-1234yf/134a	89.8/10.2	94.4	201.9
R-451B	R-1234yf/134a	88.8/11.2	94.3	201.7
R-452A	R-32/125/1234yf	11/59/30	75.1	167.1
R-452B	R-32/125/1234yf	67/7/26	77.1	170.8
R-452C	R-32/125/1234yf	12.5/61/26.5	74.1	165.3
R-454A	R-32/1234yf	35/65	81.7	179.1
R-454B	R-32/1234yf	68.9/31.1	78.1	172.6
R-454C	R-32/1234yf	21.5/78.5	85.7	186.2
R-455A	R-744/32/1234yf	3/21.5/75.5	85.6	186.1
R-456A	R-32/134a/1234ze(E)	6/45/49	102.7	216.9
R-457A	R-32/152a/1234yf	18/12/70	91.3	196.3
R-458A	R-32/125/134a/227ea/236fa	20.5/4/61.4/13.5/0.6	92.1	197.7
R-459A	R-32/1234yf/1234ze(E)	68/26/6	79.6	175.3
R-460A	R-32/125/134a/1234ze(E)	12/52/14/22	83.6	182.5
R-460B	R-32/125/134a/1234ze(E)	28/25/20/27	88.1	190.5
R-500	R-12/152a	73.8/26.2	102.1	215.7
R-501	R-22/12	75/25	95.9	204.5
R-502	R-22/115	48.8/51.2	81.5	178.7
R-503	R-23/13	40.1/59.9	18.3	64.1
R-504	R-32/115	48.2/51.8	62.2	144.0
R-507A	R-125/143a	50/50	70.6	159.1
R-508A	R-23/116	39/61	10.2	50.3
R-508B	R-23/116	46/54	11.2	52.2
R-509A	R-22/218	44/56	68.5	155.2
R-510A	DME/600a	88/12	125.7	258.2
R-511A	R-290/DME	95/5	97.0	206.6

ASHRAE Designation	Components	Composition (mass %)	T_{crit} (°C)	T_{crit} (°F)
R-512A	R-134a/152a	5/95	112.8	235.1
R-513A	R-1234yf/134a	56/44	94.9	202.8
R-513B	R-1234yf/134a	58.5/41.5	94.8	202.6
R-515A	R-1234ze(E)/227ea	88/12	108.2	226.7

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) blend 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/m³]

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

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

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

V_{liq} – liquid volume per unit mass of the blend [m³/kg]

V_{vap} – vapor volume per unit mass of the blend [m³/kg]

$Vq = V_{vap} / (V_{vap} + V_{liq})$ - volumetric quality [m³/m³]

Subscripts

vap – vapor phase

liq – liquid phase

Calculation steps

1. Calculate the saturated liquid density at T_F and the original blend composition, $\rho_{liq}(T_F)$
2. Calculate the thermodynamic state point of the blend defined by:
 - original blend 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 blend
 - liquid volume: $V_{liq}(T_L) = (1 - xq) / \rho_{liq}(T_L)$
 - vapor volume: $V_{vap}(T_L) = xq / \rho_{vap}(T_L)$
 4. Calculate the volumetric quality, $Vq(T_L)$
$$Vq(T_L) = V_{vap}(T_L) / [V_{vap}(T_L) + V_{liq}(T_L)]$$

Appendix G

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 installation, please let us know by contacting:

SRD Customer Support
National Institute of Standards and Technology
100 Bureau Drive, Stop 6410
Gaithersburg, MD 20899-6410
Tel: 1(844) 374-0183 (Toll Free)
e-mail: data@nist.gov

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

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