

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

Version 3.2

Users' Guide

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# **1. INTRODUCTION**

As alternatives to ozone depleting materials, mixtures (blends) 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. The simulation algorithms used by REFLEAK were validated against experimental results [1, 2]. Thermodynamic properties of the refrigerant mixtures are calculated using the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP): Version 8.0 [3].

#### **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 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.

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

NIST regularly updates the REFPROP database [3]. When this occurs, this simulation model will be revised to reflect the new property routines.

Compared to Version 3.1, this version of REFLEAK includes an input option for the initial volumetric quality based on the maximum liquid fill at a different fill temperature. This option is consistent with the specification of the initial volumetric quality used in ANSI/ASHRAE Standard 34 [4].

# 2. INSTALLATION

#### System Requirements

REFLEAK is designed to run on any personal computer capable of running Microsoft Windows 98, 2000, Me, XP, or similar operating system. The program requires 10 MB hard disk space.

#### 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, fluid in a vapor or liquid phase escapes from the system. In the leak process of a zeotropic 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 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) the isothermal leak and (2) the adiabatic leak. 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.

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/recharge process, the temperature in the system is "reset" to the initial temperature before the leak.

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 8.0 [3]. 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, save data, and save and/or print graphs.

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

- (1) Selecting the refrigerant blend for the leak/recharge simulation. Note: the refrigerant blend 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.
    - 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 the 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 [4]. 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 the graph indicates specific values corresponding to the xaxis 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.

- (3) Saving the output data to a specified file.
- (4) Printing the output data and/or graph.
- (5) Redrawing the graph.
- (6) 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).

#### REFERENCES

- 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 1(1), 3-20.
- [2] Kim, M.S. and Didion, D. A., 1995, "Simulation of a Leak/Recharge Process of Refrigerant Mixtures", Int. Journal of HVAC&R Research 1(3), 242-254.
- [3] 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, MD, U.S.A.
- [4] American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc., (ASHRAE), 2007, ANSI/ASHRAE Standard 34-2007, Designation and Safety Classification of Refrigerants".
- [5] McLinden, M.O., 2007, Private communication.

# 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.

Refleak 3.2		
NIST	Refleak	
	NIST Standard Reference Database 73	
NIST LEAK AN	ID RECHARGE SIMULATION PROGRAM FOR REFRIGER	ANT MIXTURES
Na	istributed by: Standard Reference Data Progran ational Institute of Standards and Technology aithersburg, MD 20899	n
David A. Didion, Min Soo K	(im and Piotr A. Domanski	Version 3.2
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quality copy of the Databa basis of sound scientific j	tandards and Technology [NIST] will use its best effo ise and to verify that the data contained therein have judgement. However, NIST makes no warranties to th age that may result from errors or omissions in the Da	been selected on the at effect, and NIST shall
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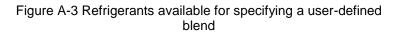
Figure A-1 Introductory screen

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. Also, the refrigerant could be specified by using the menu 'Selection/Refrigerants/Define New Blend' or by clicking the toolbar icon **S**.

😓 REFLEAK-nonamed.out		
File Selection Help		
🛎 🕺 🗱 📅		
Refrigerant	Leak/Recharge Processes	
Refrigerant		Units
Predefined Blend		View Mixing Parameters
		<u>A</u> nalyze
Define New Blend		Display <u>R</u> esults
		Vapor V Liquid
		<u>E</u> xit

Figure A-2 Main window for data entry

🔯 Define New Blend	X
Continue New Blend      Available fluids     Dutane     Dutane [1-butene]     cathon dioxide     cyclopropane     dimethylether (methoxymethane)     ethane     ethylene (ethene)     isobutane [2-methylpropane]     isobutane [2-methylpropane]	Selected blend components
Isobacter (2 methylpentane) isobexare (2 methylpentane) isopentane (2 methylputane) methane propane propane propylene (propene) R11 (trichorofluoromethane) R113 (1,1,2-trichloro-1,2-trifluoroethane) R114 (1,2-dichloro-1,2-2triefluoroethane) R115 (chloropentafluoroethane) R115 (chloropentafluoroethane) R12 (dichlorodifluoromethane) R12 (2,2-dichloro-1,1,1-trifluoroethane) R12 (2,2-dichloro-1,1,1-trifluoroethane) R12 (2,2-dichloro-1,1,1-trifluoroethane) R12 (1,2-dichloro-1,1,1-trifluoroethane)	∠dd ··> < <u>R</u> emove
	<u>D</u> K <u>C</u> ancel



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.

R12 (dichlorodifluoromethane)       R32 (difluoromethane)         R124 (1-chloro-1.1.1-urifluoroethane)       R32 (difluoromethane)         R125 (Lorotifluoromethane)       R132 (notorifluoromethane)         R1416 (1.1.dichloro-1fluoroethane)       R145 (1.1.dichloro-1fluoroethane)         R145 (1.1.dichloro-1fluoroethane)       R145 (1.1.dichloro-1fluoroethane)         R145 (1.1.dichloro-1fluoroethane)       R145 (1.1.dichloro-1fluoroethane)         R145 (1.1.dichloro-1fluoroethane)       R145 (1.1.dichloroethane)         R21 (dichlorotoromethane)       R22 (not (1.1.2.3.3.3-hextafluoropropane))         R227ea (1.1.1.2.3.3.3-hextafluoropropane)       R236 (1.1.2.3.3-hextafluoropropane)         R245 (1.1.1.2.3.3-hextafluoropropane)       R245 (1.1.1.2.3.3-hextafluoropropane)         R256 (1.1.1.2.3.3-hextafluoropropane)       R256 (1.1.1.3.3.3-hextafluoropropane)         R256 (1.1.1.2.3.3-hextafluoropropane)       R35 (1.1.1.3.3-pentafluoropropane)         R256 (1.1.1.2.3.3-hextafluoropropane)       R36 (1.1.1.3.3-pentafluoropropane)         R35 (1.1.1.2.3.3-hextafluoropropane)       R36 (1.1.1.3.3.3-hextafluoropropane)         R35 (1.1.1.3.3.3-hextafluoropropane)       R36 (1.1.1.3.3.3-hextafluoropropane)         R36 (1.1.1.3.3.3-hextafluoropropane)       R36 (1.1.1.3.3.3-hextafluoropropane)         R36 (1.1.1.3.3.3-hextafluoropropane)       R36 (1.1.1.3.3.3-hextafluoropropane)         R36 (1.1.	vailable fluids		Selected blend components	
RC318 (octafluorocýclobutane) trifluoroiodomethane	R123 (2.2-dichloro-1.1.1-trifluoroethane) R125 (pentafluoroethane) R125 (pentafluoroethane) R135 (chlorotrifluoromethane) R141 (tertifluoromethane) R141 (tertifluoroethane) R142b (1-chloro-1.1-difluoroethane) R142b (1-chloro-1.1-difluoroethane) R142b (1-chloro-1.1-difluoroethane) R142b (1-chloro-1.1-difluoroethane) R122 (chlorofluoromethane) R2152a (1.1-difluoroethane) R2152a (1.1-difluoroethane) R22 (chlorofluoromethane) R225 (tilluoromethane) R225 (tilluoromethane) R235 (tilluoromethane) R236 (1.1.1.3.3-shexafluoropropane) R245ca (1.1.2.3-a)-athexafluoropropane) R245ca (1.1.1.3.3-pentafluoropropane) R245ca (1.1.1.3.3-pentafluoropropane)			

Figure A-4 Appearance of window after selection of refrigerants

2	Specify Blend Composition			×
В	lend Name: R32/R134a			
	<u>C</u> omponents and composition Sum 1.000	Ma	ss Fraction 💌	
	R32 R134a		0.500 0.500	]
	<u>S</u> tore Info	<u>0</u> K	<u>C</u> anc	el

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'.

Save in:	🗀 Mixtures		•	← 🗈 💣 📰•	
My Recent Desktop My Documents	R32-R134a     R401A     R401B     R401B     R402B     R402A     R402A     R402A     R402A     R403A     R403A     R405A     R405A	R407C     R407C     R407E     R407E     R408A     R409A     R409B     R410A     R410B     R411A     R411B     R411A     R411A     R412A     R412A     R413A     R414A	R4148 R4158 R4158 R4164 R4174 R4184 R4194 R4204 R4218 R4220 R4218 R4228 R4228 R4222 R4222	R422D     R423A     R424A     R424A     R425A     R425A     R425A     R425A     R425A     R425A     R500     R500     R501     R502     R503     R504     R504     R504	k R508A R508B R509A steve test
My Computer	<			)	)
<b></b>	File name:			•	Save
My Network Places	Save as type:	(*.mix)		•	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.

The second secon			
File Selection Help			
🖻 🐕 🚰 📅			
Refrigeran	t Leak/Re	charge Processes	
	, <u> </u>	Ť	Units
Selection	Information		
R32-R134a(30-70)	Critical temperature: 91.5	5 °C	<u>V</u> iew Mixing Parameters
	Critical pressure: 4856	.4 kPa	
Refrigerant	Breakdown		<u>A</u> nalyze
Predefined Blend	<u>ا</u>	Mass Fraction 💌	
	Component	Composition	Display Results
	R32	0.300	Disbink Teaning
	R134a	0.700	✓ Vapor ✓ Liquid
Define New Blend		·	j <b>⊘</b> Liquia
			<u>E</u> xit

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

REFLEAK-nonamed.out		
Refrigerant	Leak/Recharge Processes	Units
<ul> <li>Isothermal (slow leak)</li> </ul>	Leak Process Only	<u>V</u> iew Mixing
C Adiabatic (fast leak)	C Leak and Recharge Process	Parameters
Leaking Phase • Vapor Phase C Liquid Phase	Recharge Process           Number of recharges           % mass loss for recharging	Analyze
Initial Leak Condition	25.00 (°C)	Display <u>R</u> esults
Initial Volumetric Quality:	0.200 (fraction)	🔽 Liquid
Optional Calculation of Initial V	olumetric Quality at 25.00 ( 'C)	
Fill Temperature:	('C')	<u>E</u> ×it
Fraction of Max. Liquid Fill:	(fraction) Calculate	

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.

REFLEAK-nonamed.out		
File Selection Help		
🗃 🔀 📅		
Refrigerant	Leak/Recharge Processes	
<ul> <li>Leak Type</li> <li>Isothermal (slow leak)</li> <li>Adiabatic (fast leak)</li> </ul>	Simulation • Leak Process Only C Leak and Recharge Process	<u>U</u> nits View Mixing Parameters
C Vapor Phase C Liquid Phase C Initial Leak C	quality must be a numeric value between 0 and	Analyze           Analyze           1.           Display Results
Initial Temperature: Initial Volumetric Quality: Optional Calculation of Initial Volu	25.00 ( 'C) a (fraction) umetric Quality at 25.00 ( 'C)	Vapor Liquid
Fill Temperature:	('C) (fraction) <u>Calculate</u>	<u>E</u> xit

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, after which Figure A-10 will appear.

Refrigerant	Leak/Recharge Processes	
Leak Type	Simulation	<u>U</u> nits
Isothermal (slow leak)	Leak Process Only	View Mixin
Adiabatic (fast leak)	C Leak and Recharge Process	Parameter
Leaking Phase	Recharge Process	
Vapor Phase	Number of recharges	Analyze
C Liquid Phase	% mass loss for recharging	
Initial Leak Condition		Display <u>R</u> esu
Initial Temperature:	25.00 ( <sup>'C</sup> )	Vapor
Initial ∀olumetric Quality:	(fraction)	IV vapor IV Liquid
Coptional Calculation of Initial V	olumetric Quality at 25.00 ( 'C)	
Fill Temperature:	25.00 ('C)	Exit
Fraction of Max. Liquid Fill:	0,759 (fraction) Calculate	

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

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.

<u>U</u> nits <u>V</u> iew Mixin Parameter
<u>⊻</u> iew Mixin
Parameter
Analyze
Display <u>R</u> esu
Vapor
l⊽ Liquid

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 multi-component 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.

Mixing Parameters		
Mixing Parameters Refrigerants R32 R134a	Mixing Model [LJ5 Lemmon & Jacobson model for the F Refriger ant-Refriger ant	R32/134a miidur ▼
Zeta	R32 - R134a       vfault values should be used unless new da       xi     Fpq       12039     1	Gamma 1
	R.T.,"Equations of State for Mixtures of R-32 -152a,"J. Phys. Chem. Ref. Data, Volume 3:	
		<u>о</u> к

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

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-14). Consistent units can be selected by pressing 'SI' or 'I-P (Inch-Pound)'.

: Units		×
Dimension	Units	Design the line
Temperature	'C 🗸	Reset Units
Pressure	kPa 🗸	<u><u>S</u>I</u>
Volume	m^3 -	I-P (Inch-Pound)
Mass	kg 🗸	
,		<u>O</u> K <u>C</u> ancel



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

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.

**REFLEAK 20** 

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.

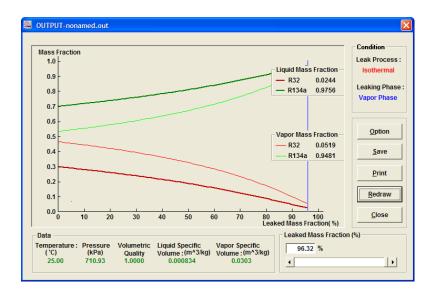


Figure A-15 Data display in a graph format (leak process)

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

Output Option	
Y Data Mass Fraction Temperature Pressure	Limits Y Range Auto Maximum 1.0 F Minimum 0.0 F
Show Mass Fractions Liquid Phase Vapor Phase	Mass Fractions Display Location <ul> <li>Automatic Display</li> <li>Right Hand Side of Data Point</li> <li>Left Hand Side of Data Point</li> </ul>
	<u>O</u> K <u>C</u> ancel

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.

## 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.

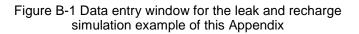
Select the icon in the program window, and then double click the REFLEAK icon.

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.

e Selection Help		
ž 🐕 🔀 📅		
Refrigerant	Leak/Recharge Processes	
- Leak Type	- Simulation	Units
<ul> <li>Isothermal (slow leak)</li> </ul>	C Leak Process Only	<u>V</u> iew Mixing
C Adiabatic (fast leak)	• Leak and Recharge Process	Parameters
Leaking Phase	Recharge Process	
Vapor Phase	Number of recharges 3	<u>A</u> nalyze
C Liquid Phase	% mass loss for recharging 30.0	
Initial Leak Condition		Display <u>R</u> esults
Initial Temperature:	25.00 ('C)	Vapor
Initial Volumetric Qualitγ:	0.200 (fraction)	Vapor
Optional Calculation of Initial	Volumetric Quality at 25.00 ( 'C)	
Fill Temperature:	('C)	<u>E</u> xit
Fraction of Max. Liquid Fill:	(fraction) Calculate	



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).

			<<	L	E	A .	К	' R	E	СH	A	R	G	E	S	I	1 U	Γſ	A T	Ι	0 N >>			
ŧ	of	RCG		0	Le	ak	ed	fr	act	ion	¢,	mas	s	• =	1 2 3	. 00; . 00; . 00;	~ ~ ~ ~	(mo:	le)		0.00% 1.12% 2.24% 3.36%	VQ	0.2500 0.2582 0.2664 0.2745	
ŧ	of	RCG		Ø	Le	ak	ed	fr	act	ion	¢,	mas	s	• :	5 6 7	(00 (00) (00) (00) (00)		(mo:	le)		4.48% 5.60% 6.71% 7.83% 8.94%	ŲQ	0.2827 0.2908 0.2990 0.3071 0.3153	
Ħ	of	RCG		0	Le	ak	ed	fr	act	ion	۲,	mas	s	• =	9 10 11 12	.00;		(mo:	le)		10.05% 11.16% 12.26% 13.37% 14.47%	ŲQ	0.3234	
Ħ	of	RCG		Ø	Le	ak	ed	fr	act	ion	¢,	mas	s)	• :	15 16 17	00: 00: 00: 00: 00:		(mo:	le)		15.57% 16.67% 17.77% 18.87% 19.96%	ŲQ	0.3640 0.3722 0.3803 0.3884 0.3864	
Ħ	of	RCG		Ø	Le	ak	ed	fr	act	;ion	G	nas	s)	) :	19	.00;		(mo:	le)		21.06× 22.15×	ŲQ	0.4045	

Figure B-2 Progress of simulation for a leak and recharge process

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

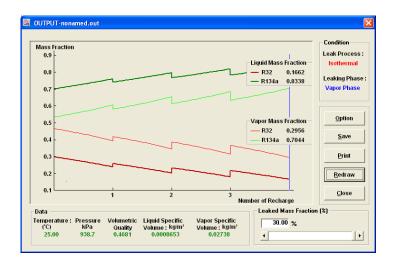


Figure B-3 Data display in graphical format (leak and recharge process)

# 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>lcon</u>	Equivalent File Option	Functions and Uses
ß	<u>O</u> pen	Open <b>the file saved in a</b> previous process
	<u>S</u> ave	Save the current process
4	<b>P</b> rint	Print <b>output</b>
**	Predefined Blend	Specify predefined blends
**	<u>D</u> efine Blend	Specify user-defined blend
	Output	Display output
	Units	Selection of units

# Appendix D

# SINGLE-COMPONENT REFRIGERANTS AVAILABLE IN REFLEAK

Short Name		Full Chemical Name
R11 R113 R114 R115 R116 R1150 R12 R123 R124 R125 R1270 R13 R134a R14 R141b R142b R143a R152a R170 R21 R218 R22 R227ea R23 R236ea R236fa R245ca R236fa R245ca R236fa R245ca R245fa R290 R32 R365mfc R41 R50 R600	or propylene or isobutane	trichlorofluoromethane 1,1,2-trichloro-1,2,2-trifluoroethane 1,2-dichloro-1,1,2,2-tetrafluoroethane chloropentafluoroethane ethylene dichlorodifluoromethane 1,1-dichloro-2,2,2-trifluoroethane 1-chloro-1,2,2,2-tetrafluoroethane pentafluoroethane propene chlorotrifluoromethane 1,1,2-tetrafluoroethane 1,1-dichloro-1-fluoroethane 1,1-dichloro-1-fluoroethane 1,1-dichloro-1-fluoroethane 1,1-difluoroethane 1,1-difluoroethane 1,1,1-trifluoroethane 1,1,1,2,3,3-heptafluoropropane trifluoromethane 1,1,2,3,3-heptafluoropropane 1,1,3,3-pentafluoropropane 1,1,3,3-pentafluoropropane 1,1,1,3,3-pentafluoropropane 1,1,1,3,3-pentafluoropropane 1,1,1,3,3-pentafluoropropane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane 1,1,1,3,3-pentafluorobutane fluoromethane methane butane 2-methylpropane carbon dioxide
RC318		octafluorocyclobutane

E170	or dimethylether e	ethylene oxide
C4H8		butene
C3H6		cyclopropane
C4H8	or isobutene	2-methyl-1-propene
C6H14	or isohexane	2-methylpentane
C5H12	or isopentane	2-methylbutane
C5H12	•	pentane
CF3I		trifluoroiodomethane

# Appendix E

# PREDEFINED REFRIGERANT MIXTURES AVAILABLE IN REFLEAK

	<b>a</b>	
ASHRAE	Composition	Mass
<b>Designation</b>	<u>Components</u>	Percentages
D 401 A	R22/152a/124	E0/40/04
R401A R401B	R22/152a/124 R22/152a/124	53/13/34 61/11/28
	R22/152a/124 R22/152a/124	
R401C		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
	11120/1010/0000	55.1/ T 1.0/0.7

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
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

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

For fractionation analysis, ANSI/ASHRAE Standard 34 [4] 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 [5].

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:

 $\begin{array}{l} \rho - \text{density [kg/m^3]} \\ m_{\text{liq}} - \text{mass of refrigerant liquid [kg]} \\ m_{\text{vap}} - \text{mass of refrigerant vapor [kg]} \\ xq = m_{\text{vap}} / (m_{\text{vap}} + m_{\text{liq}}) - \text{vapor quality [kg/kg]} \\ V_{\text{liq}} - \text{liquid volume per unit mass of the mixture [m^3/kg]} \\ V_{\text{vap}} - \text{vapor volume per unit mass of the mixture [m^3/kg]} \\ Vq = V_{\text{vap}} / (V_{\text{vap}} + V_{\text{liq}}) - \text{volumetric quality [m^3/m^3]} \end{array}$ 

<u>Subscripts:</u> vap – vapor phase liq – liquid phase

#### Calculation steps:

- Calculate the saturated liquid density at T<sub>F</sub> and the original mixture composition, pliq(T<sub>F</sub>)
- 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  $F_{\rm F} \cdot \rho_{\rm liq}(T_{\rm F})$

Results:

- saturated vapor density at the coexisting vapor composition,  $\rho_{vap}(T_L)$
- saturated liquid density at the coexisting liquid composition,  $\rho_{\rm liq}(T_{\rm L})$
- vapor quality, xq
- 3. Calculate the liquid and vapor volumes per unit mass of the mixture

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

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

 $Vq(T_{\rm L}) = V_{\rm vap}(T_{\rm L})/[V_{\rm vap}(T_{\rm L}) + V_{\rm liq}(T_{\rm L})]$ 

## 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:

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