Sources of refrigerant property data

Traditionally most of the needed refrigerant properties could be found in the tables and plots listed in refrigeration books. With current pace of refrigerant development, there is a need to get property data of ever growing amount of new refrigerants. This is when the electronic property databases comes handy. In this article we will review some of the databases available.

Refrigerant properties

Various refrigerants have different properties that greatly influence the refrigeration system design and performance. To design a specific refrigeration system one relies on a set of thermodynamic property data that is often found in specific refrigerant property databases. But where does this data come from?

While it is possible to measure some thermodynamic properties of a given fluid (as for instance temperature and pressure), there are a number of properties that cannot be directly measured (e.g. enthalpy) and therefore calculated using certain thermodynamic relations. The relation between thermodynamic properties at a specific state is known as equation of state (denoted as EoS).

Pv=Rt is an example of an equation of state of an ideal gas. Real fluids often cannot be approximated to be considered as ideal gases and therefore more complex EoS used. Most current refrigerants are described by EoS built based on Helmholtz energy formulations. The form of such EoS normally relies on a limited amount of experimentally obtained properties. The information about the EoS used to describe a certain substance is normally referred in the available databases (Figur 1).

R1234ze(E) - CHF=CHCF3 (trans) - trans-1,3,3,3-tetrafluoropropene (CAS# 29118			
Molar mass Trip 114,04 kg/kmol 11	le pt. temp. Normal 68,62 K 254,	Gaspha coiling pt. dipole at l ,18 K 1,27 det	ase NBP oye
Critical Point Temperature F 382,51 K 3,6	Pressure De 1349 MPa 489,24	nsity Acentric f. I kg/m³ 0,313	actor
Range of applicability Minimum temp. Maxi 168,62 K	imum temp. Maximun 420, K 20,	n pressure Maximum o MPa 1512,2 kg	density g/m³
NIST Rec: FEQ_Helmholtz equation of state for R1234ze of Thol and Lemmon (2013). LITERATURE REFERENCE Thol, M. and Lemmon, E.W. to be published in Int. J. Thermophys., 2013. The uncertainty in density in the liquid phase of the equation of state is 0.1% from 200 K to 380 K and pressures up to 40 MPa. The uncertainty increases outside of this region and in the vapor phase to 0.5%, and even higher in the critical region. In the gaseous region, the speed of sound can be calculated with an uncertainty of 0.05%. In the liquid phase, the			
Equation of State Viscosity		<u>Ihermal Conductivity</u>	
Surface tension <u>M</u> elting Line		Su <u>b</u> limation Line	
<u>O</u> K <u>C</u> ancel	Print	Сору С	opy <u>A</u> ll

Figur 1 – Example of EoS data for a refrigerant in Refprop 9.1 database

Reliable EoS require reliable input properties. The challenge with new refrigerants' properties is that the quality measured data is often not available at an early stage of development and therefore such new substances are often missing from databases. There is, however, possibly to define such new substance using simplified EoS and limited amount of properties (as little as just the structural form of molecule and its natural boiling point) [1]. While such methods are not providing exact property data, such properties can still be used provided one is aware of the uncertainties of such data.

REFPROP

REFPROP [2] is perhaps the most known and the most used fluid thermodynamic and transport properties database out there. It is developed by NIST, the U.S. National Institute of Standards and Technology.

The property data can be accessed directly through the graphical interphase, or indirectly from a number of supported environments as for instance Excel, Mathlab and Python. The graphical interphase provides good functionality and have many useful functions as for instance plotting the property diagrams and generating property tables. For complete set of functionality one can refer to the REFPROP manual [3]. Fully functional free REFPROP version with very limited set of fluids is also available [4].

The number of fluids supported by the latest REFPORP 9.1 is greater than a hundred and includes such new refrigerants as R1234yf and R1234ze(E). As the program cannot be automatically updated, the new fluids are often published online [REF]. For instance it is now possible to add support to such new refrigerants as R1234ze(Z) and R1233zd(E) by downloading respective files. When such updates are not available, it is still possible to user define a substance by providing a set of known data. In this case the user should be aware on the uncertainty the calculated properties can have when using this method.

Many new refrigerants are mixtures of a few substances. REFPROP offers possibility to select a mixture from a list of predefined mixtures or define a new one based on the mixture composition. A number of new refrigerant mixtures that is not predefined in original REFPROP 9.1 is available for download from their website [5]. This update includes many new refrigerant mixtures (e.g. R449A, R448A, R452A, R513A) and is constantly updated, with the most recent additions this year being refrigerants R449B and R454A.

When calculating properties of a refrigerant mixture REFPROP relies on specific mixing parameters that are listed in a special text file (HMX.BNC). For a number of new mixtures that contain HFOs the mixing parameters were not defined until recently. Now it is possible to request the updated HMX.BNC file and reliably predict mixtures as for instance such as R448A that consist of fluids R32, R125, R134a, R1234yf, and R1234ze(E). It should be noted that without replacing the HMX.BNC file with its new version REFROP will not calculate the properties of such new mixtures correctly.

Coolprop

Coolprop [6] is a closest alternative to REFPROP. In fact, it was developed with some input from Eric Lemmon [6], the person behind the development of REFPROP. Unlike REFPROP, it is not a standalone program, but rather a thermodynamic and transport properties library, that should be accessed from other programs. The list of supported programs and environments is constantly updated and now include the majority of programming languages and platforms of technical interest as EES, Excel, Matlab, Python and etc. There is also web interface under development.

The amount of fluids included in Coolprop is similar to that included in REFPROP. The major difference here is that there is limited possibility to work with refrigerant mixtures. Some common refrigerant mixtures are presented in the list of fluids, and there is limited possibility to user define mixtures. But defining the mixtures of many new refrigerant is impractical, as can only be done by imputing a set of data describing interaction behavior for mixture components.

The major advantage of the Coolprop is that it is an open-source software that is free to download and use. In return the developers ask a user to make a reference to CoolProp if it is used in an academic work.

Other sources

Another source of refrigerant property data are the refrigerant manufacturers themselves. For instance, two major refrigerant manufacturers – Honeywell and Chemours – each offer tools to obtain refrigerant property data. DUPREX [7] is the tool provided by Chemours. In addition to a number of convention refrigerants, as R134a and R404A, the tool provides data on properties of several new refrigerants as for instance R449A, DR-7, DR-5 and etc.

Genetron Properties [8] is a similar program from Honeywell. Both programs provides similar functionality. In adition to the refrigerant property data, both programs offer cycle evaluation functionality where user can select on of a few predefined cycles and calculate necessary parameters. While somewhat similar, Genetron Properties has greater functionality compared to Duprex as has greater amount of predefined cycles and greater functionality when working with refrigerant properties.



User interfaces of DUPREX and Genetron Properties are presented on Figures 2 and 3 respectively.

Figur 2 – DUPREX user interface



Figur 3 – Genetron Properties user interface

While there are a number of smaller softwares that provide access to refrigerant properties, there is only one that we will mention here Engineering Equation Solver (EES). EES is known software that gained its popularity partly due to the property data that is embedded into the software. As for the refrigerants, it contains a list of refrigerants, including new ones. Moreover, current version of the EES provides aces to R1243zf property data, unlike any other software discussed here. The list of supported refrigerant mixtures is hovewer limited to a few refrigerants.

The described software cover a wide range of needs when it comes to obtaining refrigerant properties. REFPROP is still state of the art in the field of calculating property data. It strongest competitive advantage is its comprehensive functionality and ability to calculate property data of many new refrigerant mixtures. Coolprop is the only software that can be considered as an alternative to REFPROP. While having somewhat limited functionality due to the absent of graphical interphase, it has an advantage of being free open-source software, thus having all prerequisites to be developed further. We As it comes to the software from refrigerant manufacturers, it can be considered as a source of reference property data, especially when it comes to the properties of new refrigerant mixtures. As a bonus, embedded refrigeration cycles make them very useful when in need of a quick check.

Följ gärna våra publikationer och få vårt digitala nyhetsbrev. Anmäl dig genom att följa länken bit.ly/kth_ett.

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