

Properties of the substances: from a special program to the functions of the mathematical package

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At the present time the technical and engineering evaluations are more often made in *mathematical packages* such as Mathcad, Matlab, Maple, Mathematica rather than using programming languages (C, BASIC, Pascal, etc.) that enables us to speed-up the development of evaluation by an order. The efficiency of the evaluations will increase if the mathematical packages are equipped with functions returning *properties of the substances and materials* used in evaluations. Usually such properties are computed by the special programs. One of the most powerful program of such type is REFPROP (www.nist.gov/srd/nist23.htm – [1]) by National Institute of Standards and Technology. It represents thermal physical properties of basic substances and their mixtures used in industries as separate values, tables (numerical arrays) and plots. The main limitation of this and the similar programs is that the generated data (properties of substances) could be transferred into separate engineering and technical evaluations only *manually*. REFPROP and “the same programs” don’t generate functionalities visible in “the separate engineering and technical evaluations” that make them difficult to use in the mathematical programs and engineering calculators. The way to eliminate this disadvantage is described below: how to generate not only separate numbers and tables (numerical arrays) but also functions of substance properties using such programs as REFPROP.

Fig. 1 shows the initial dialog of a user with REFPROP program: the about box, Substance menu by which a REFPROP user specifies certain thermal and physical properties.

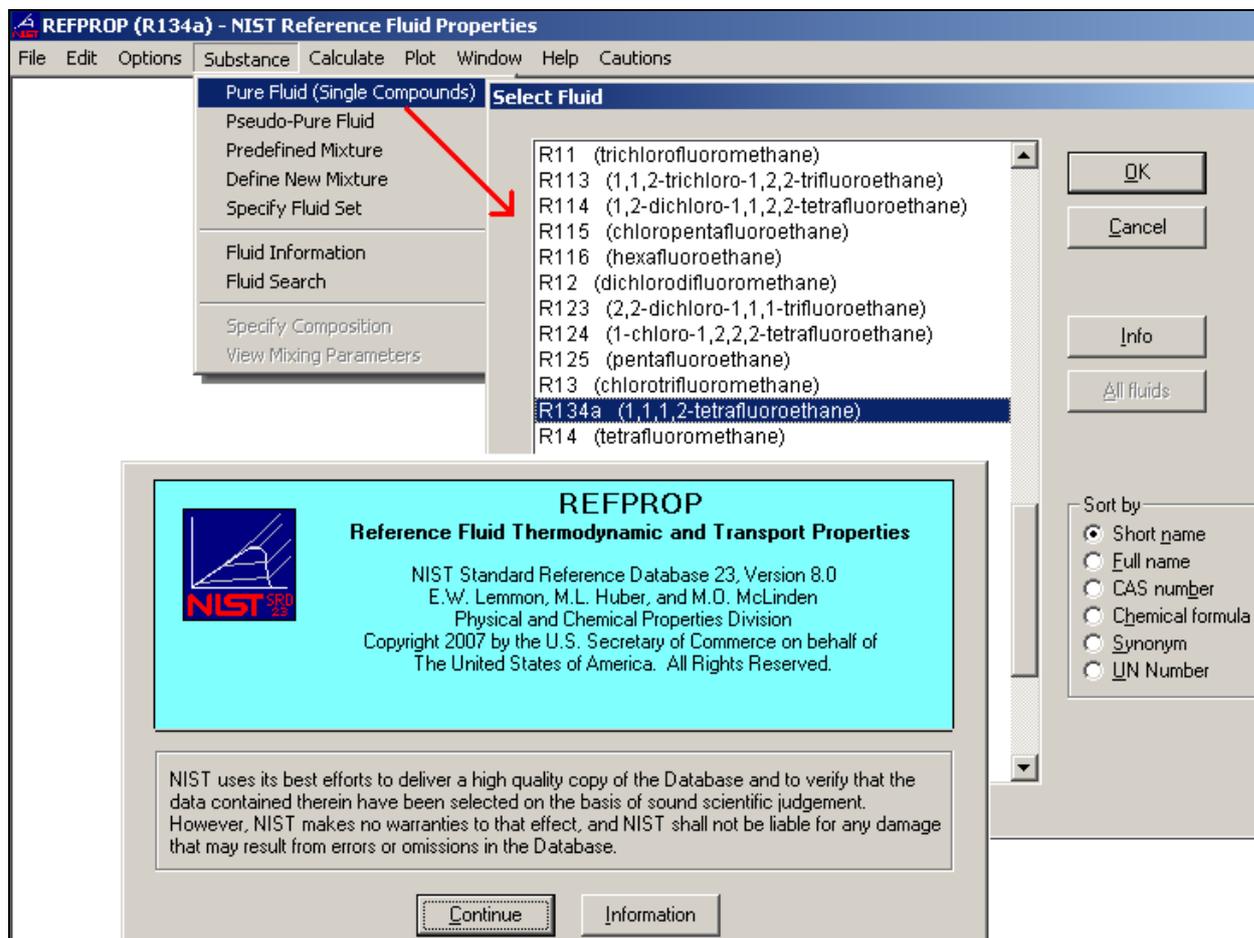


Figure 1. The dialog of choosing the substance in REFPROP program

The list of properties of the chosen substance, their dimensions, and also format of the number (significant values et al.) are defined by commands **Properties**, **Units** and **Preferences** (which are not represented on Fig 1) of the **Options** menu (left to the **Substance** menu).

Having chosen the substance (Fig. 1¹) one can calculate its thermal and physical properties that is represented on the next figure. Fig. 2 shows **Calculate** menu and the table obtained by command **Saturation Point**.

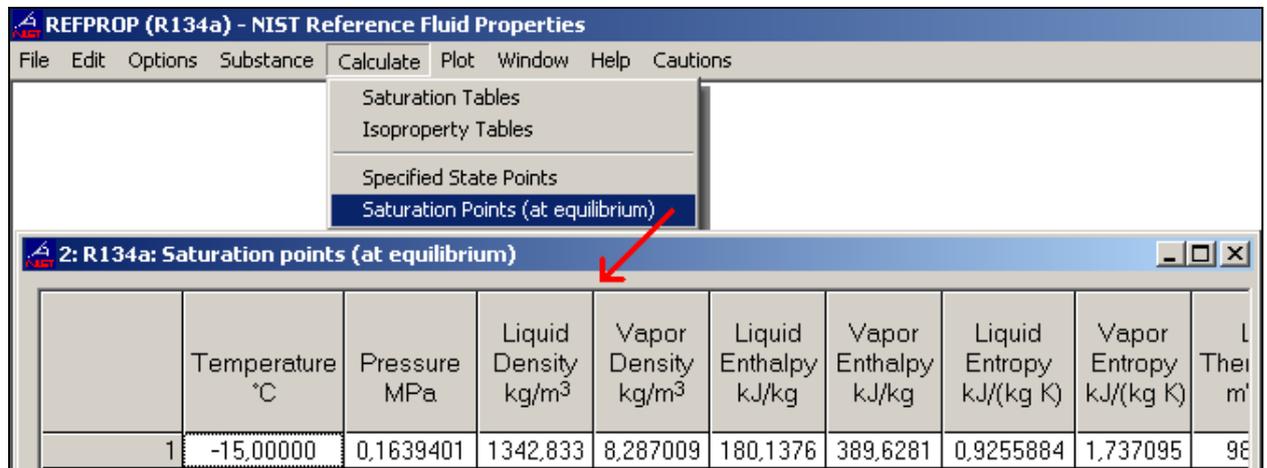


Figure 2. Dialog of calculation of the substance thermal physical properties in REFPROP program

A user of REFPROP can enter a parameter of the substance (temperature or pressure, density of the liquid or density of steam at the saturation line), click **Enter** button and get remaining calculated properties of the chosen substance. At that, an empty row for a new user request will appear below the current table row shown on Fig. 2.

Thus, entering a parameter and obtaining the remaining calculated parameters (properties) a user forms a table (numerical array) of the substance properties with arbitrary variation value of the parameter, for example, temperature. For the fixed variation value it is possible to complete the table of the substance properties at the saturation line automatically by command **Saturation table** from the **Calculate** menu, see Fig. 3.

¹ It was chosen the cooling agent R-134a (1,1,1,2-Tetrafluoroethane)

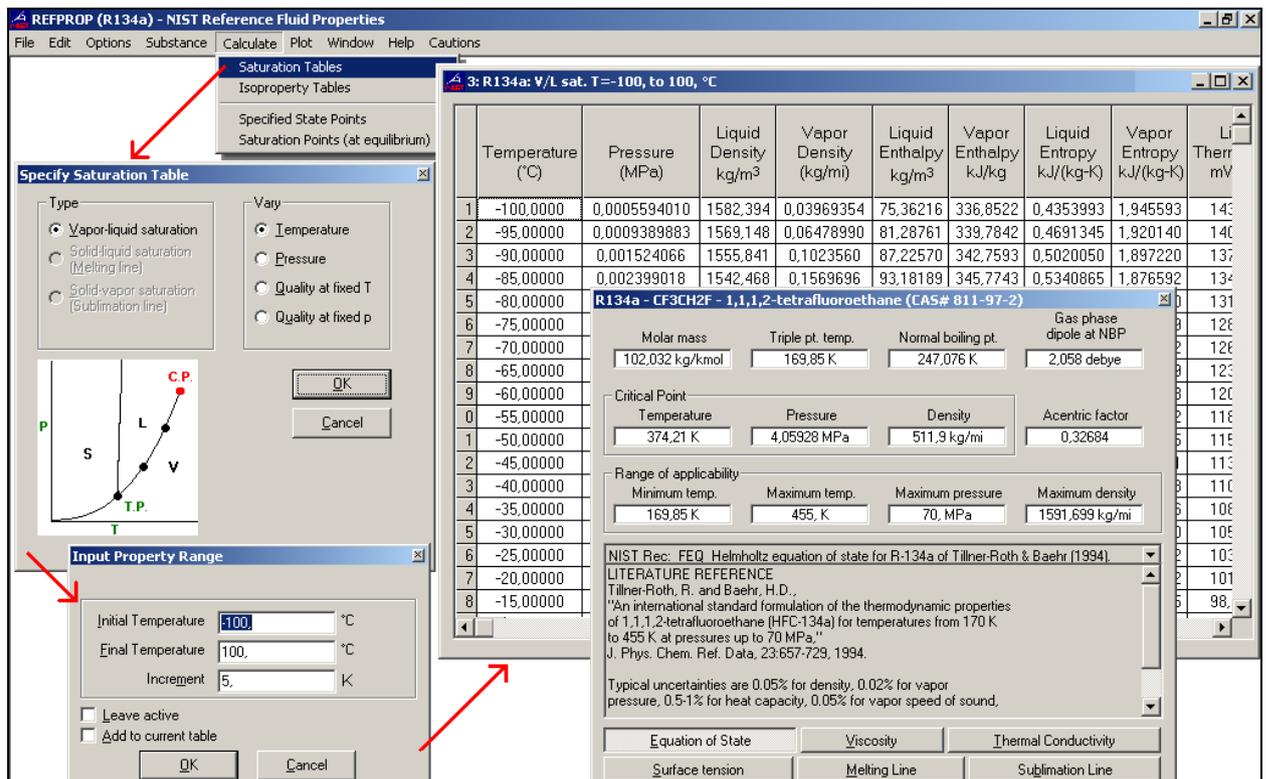


Figure 3. The dialog of creating a table of the substance properties at the saturation line in REFPROP

Figure 3 shows the REFPROP dialog for obtaining a table of properties of R-134a cooling agent at the saturation line for temperature range varying between minus 100°C to 100°C with step of 5K. Additionally, the dialog box containing data on the substance and the literature reference for calculation formulae is represented over the table on Fig. 3. The dialog box is called up by command Fluid information from the **Substance** menu. This “information” is discussed below (see Fig. 6).

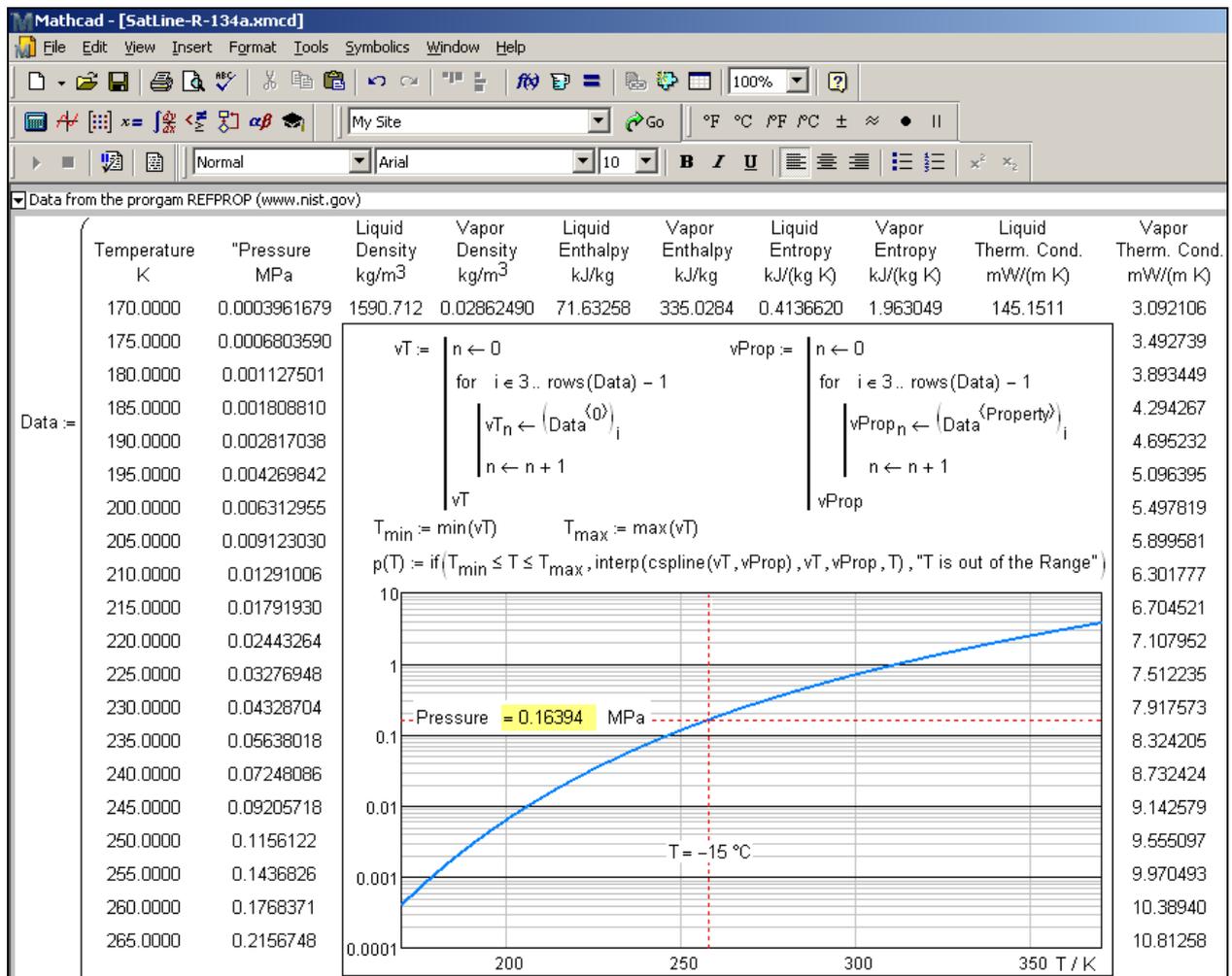
Separate values, tables, and plots (the **Plot** menu is used to create plots in REFPROP, see Figures 1-3) are appropriate for *manual* calculations, step-by-step engineering calculations by calculators or with the help of a slide rules (let’s recall a precomputer era), whereby the required values are taken from the reference books (at once or after a certain interpolation) or from the plots². As a rule, scientific and technical calculations of such type are now made not manually but with the help of programs, which are developed by engineering technicians or are acquired from third-party designers. Tables and plots are not suitable for such programming calculations. In this case it is required *programmed functionalities* in which one enters initial data (the argument, for example, temperature) and gets calculated value, for example, saturated pressure.

Imagine, that an engineer is to design a cooling installation with cooling agent R-134a (1,1,1,2-Tetrafluoroethane), calculation of its properties is shown on Fig. 1-3, for example, in Mathcad. Besides Mathcad, the engineer should install REFPROP program on his computer.

² A great number of reference books include large-size diagrams with fine grids. Tolerably exact values are obtained from such diagrams without additional interpolations, inevitable while using tables. Besides, such diagrams can be used to represent various processes, for example gas throttling.

Unfortunately, there is no direct data exchange between Mathcad and REFPROP³. As a result, the engineer has to copy initial data from Mathcad manually (for example, temperature), transfer it into REFPROP, make required calculations, and return the result by copying and inserting data (for example, saturation pressure of the cooling agent) back into Mathcad.

Certainly, it would be convenient to enter the source formula⁴ for saturation pressure of cooling agent R-134a depending on temperature into Mathcad. But REFPROP program represents only reference to the described formula, rather than the formula itself. Surely, one can find the literature, take required formula, and programme it... Although, there is another way: to transfer (copy and insert) the table on the cooling agent at the saturation line from REFPROP into Mathcad and create (reconstruct) required function, see Fig. 4.



³ Such automated data exchange is performed between Mathcad and Excel. Mathcad and REFPROP developers should consider such integration in future. Now system XProps (<http://www.thermalanalysispartners.com/xprops.php>) provides such integration through DLL protocol. But this protocol won't work in the next Mathcad version (Mathcad Prime). This emphasizes topicality of suggested solutions. There is the DLL-connection between REFPROP and Mathcad from NIST. But this tools has big contingencies too.

⁴ In fact, it was done in programme WaterSteamPro (www.wsp.ru – [2]) that provides well-known calculation environments (mathematical packages, electronic tables, programming languages) with functions of thermal physical properties of the basic working media for power engineering. WaterSteamPro calculates these properties by the source formulae (formulations of the International Association for the Properties of Water and Steam - www.iapws.org).

Figure 4. Creation a function that returns saturation pressure depending on temperature in Mathcad

Mathcad includes functions (built-up functions) that enable us to make, for example, spline interpolation of table data. Figure 4 shows creating of function $p(T)$ that returns pressure depending on temperature. It is based on the built-in Mathcad functions **interp** (interpolation) and **cspline** (coefficients of the cubic spline). At that, the programme controls that entered temperature corresponds the range defined by the table. Otherwise interpolation would turn into extrapolation entailing the error⁵. As a rule, errors or uncertainties are represented in REFPROP (see dialog box containing information on the substance shown on Fig. 3). It is possible to display corresponding uncertainty of Mathcad function and, if necessary, to calculate additionally its absolute value and acceptable range of dispersion for calculated pressure.

In the Mathcad document created by this procedure a user enters temperature and choose necessary property of the substance (variable **Property**, See Fig. 4). The program will choose required columns (vectors vP and vP_{rop}) from the table (matrixes, see Fig. 4) to perform spline interpolation. Such Mathcad document can be published on the Internet by Mathcad Calculation Server technology [3] for interactive network use⁶, see Fig. 5.

⁵ Sometimes this restriction should be lifted to make extrapolation by function **interp**. For example, it is necessary to remove the restriction for the inverse problem solving by method of successive approximations, defining temperature by pressure.

⁶ Some legal issues arise here. Is REFPROP program purchased for personal use or for an enterprise? May data obtained by REFPROP be published on the Internet? It turns out that the program will be also used by those who have not acquired it.

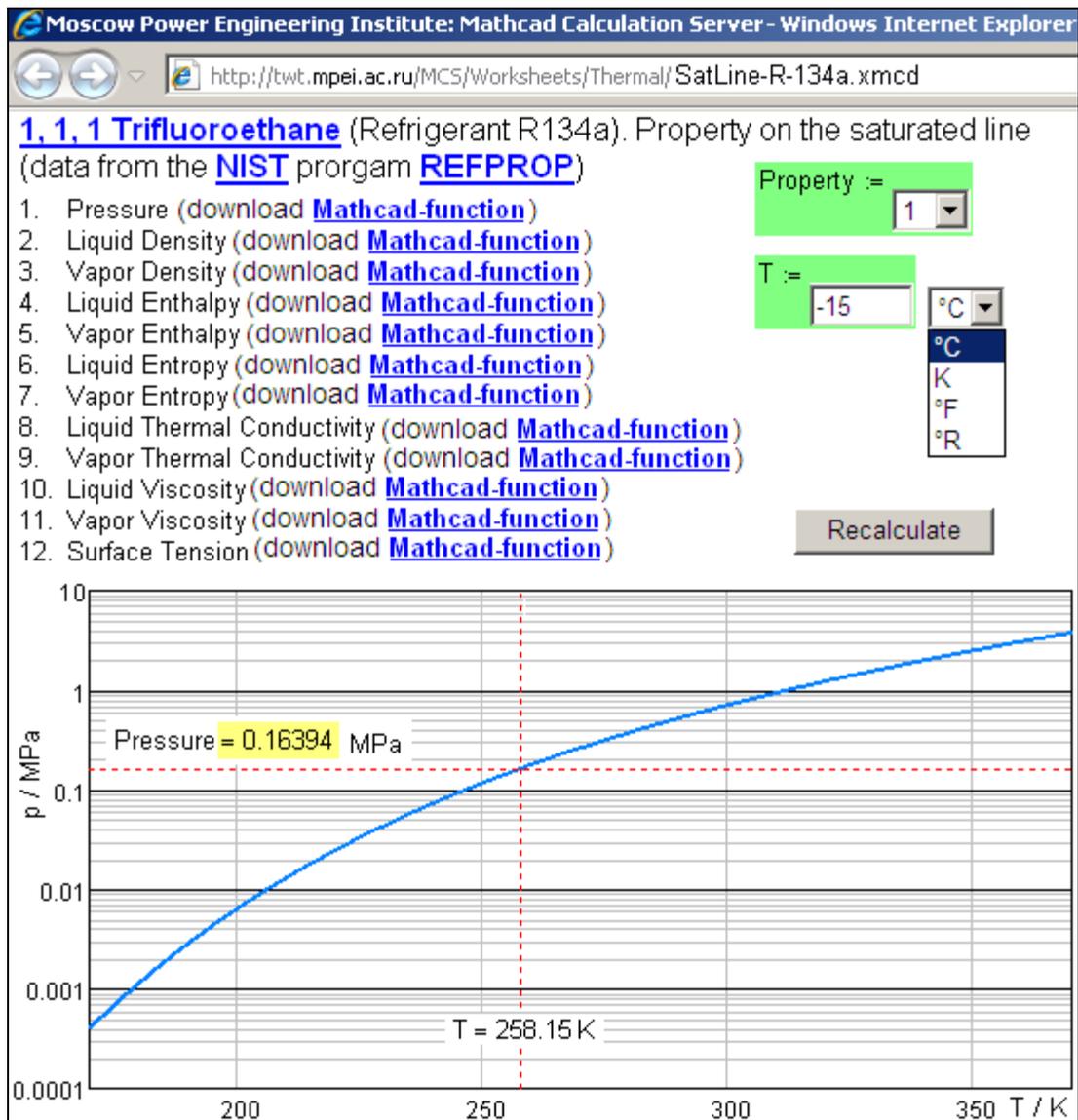


Figure 5. Network interactive calculation of cooling agent R-134a properties at the saturation line

A visitor of the site shown on Fig. 5 chooses the property of cooling agent R-134a (variable **Property**), enters temperature, clicks appropriate temperature unit (degrees Celsius, Kelvin, Fahrenheit, or Rankine) and Recalculate button, and obtains not only saturated pressure expressed in megapascals⁷ but also plot of this quantity depending on temperature with a fixed calculated point. The plot supplemented the calculation shown on Fig. 5 enable a user to see the type of the curve and permissible range of temperature changing. The similar sites have been developed for the other cooling agents included into REFPROP program. To choose the cooling agent one can visit the site <http://tw.t.mpei.ac.ru/TTHB/tthb.html> (online version of the reference book "Thermotechnics and thermal engineering"), containing the list of the cooling agents in section "Thermodynamics" and choose the substance, or just type required address changing characters R-134a in the address shown

⁷ The calculation could be performed in such a way than a user choose unit for calculated pressure: MPa, atm, psi, ksi, etc.

on Fig. 5 to the other (for example, if it is required to work with cooling agent R11 the characters should be changed to R-11).

The calculation shown on Fig. 5 contains hyperlinks (underlined texts). Where do they lead? Firstly, it is possible to go to the site in which the cooling agent (1,1,1,2-Tetrafluoroethane) is described, Wikipedia (<http://en.wikipedia.org/wiki/1,1,1,2-Tetrafluoroethane>), see Fig. 6. Wikipedia is an online encyclopedia and every viewer can introduce his own supplements and corrections. The authors of this article took the opportunity and inserted the corresponding link from Wikipedia to the calculation, see the line having mark “New”.

1,1,1,2-Tetrafluoroethane - Wikipedia, the free encyclopedia - Windows Internet Explorer

W <http://en.wikipedia.org/wiki/1,1,1,2-Tetrafluoroethane>

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1,1,1,2-Tetrafluoroethane

From Wikipedia, the free encyclopedia

1,1,1,2-Tetrafluoroethane, **R-134a**, **Genetron 134a**, **Suva 134a** or **HFC-134a**, is a **haloalkane refrigerant** with thermodynamic properties similar to **R-12** (dichlorodifluoromethane), but with less **ozone depletion potential**. It has the formula CH_2FCF_3 , and a **boiling point** of -26.3 °C (-15.34 °F).

Contents [hide]

- 1 Uses
- 2 History
- 3 Safety
- 4 References
- 5 See also
- 6 External links

Uses [edit]

1,1,1,2-Tetrafluoroethane	
IUPAC name [hide]	1,1,1,2-Tetrafluoroethane
other names [hide]	Genetron 134a HFA-134a HFC-134a R-134a Suva 134a Norflurane
Identifiers	
CAS number	811-97-2 ✓
EC number	212-377-0

External links [edit]

- The Coexisting Curve of the Refrigerant HFC 134a: Some Scaling Models
- R134a 2 phase computer cooling
- Refrigerant R134a: Property on the saturated line (on-line calculation) **New**

Figure 6. The Wikipedia page with the article concerning cooling agent R-134a

If an engineer types the key word “Refrigerant R-134a” in Google search box he (she) will see corresponding Wikipedia article and, if necessary, will go to the calculation site shown on Fig. 5. What are the other hyperlinks on the site shown on Fig. 5? Certainly, there are links to the REFPROP program,

the data source for our calculations, and to the NIST site, where the REFPROP program was created. Besides, (the key point) there are links to the server in which a visitor can download corresponding functions for Mathcad. Figure 8 shows a function of this type.

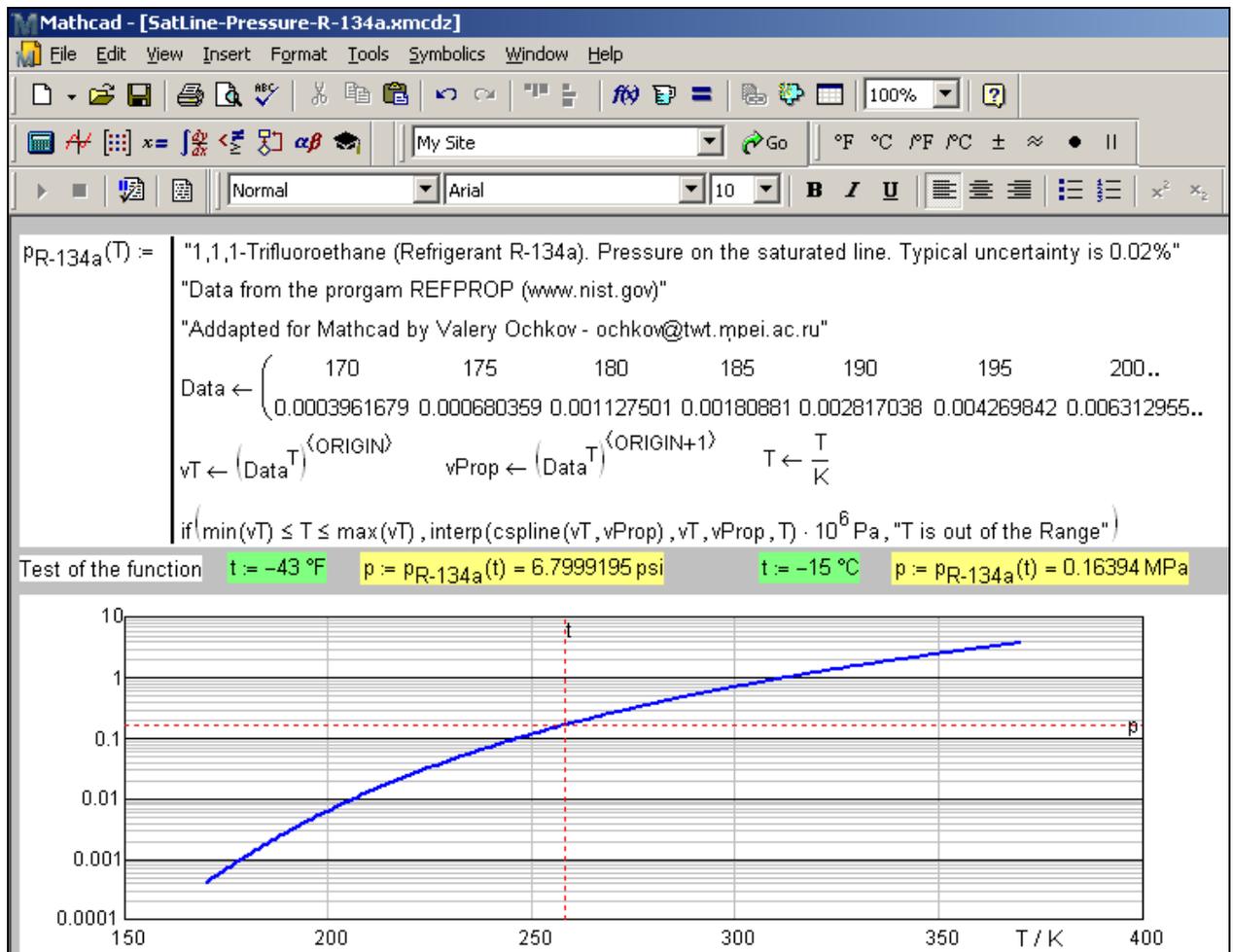


Figure 7. Mathcad function returning saturation pressure of cooling agent F134a

The base of the function shown on Fig. 7 is a matrix of two rows containing temperature and pressure values of cooling agent R-134a at the saturation line. The data have been generated by REFPROP program or have been taken from the Mathcad matrix shown on Fig. 4. This matrix is divided into two vectors vT and vP used for spline interpolation. Function $P_{R-134a}(T)$ generated in this case operates dimensional values: its argument is temperature and it returns pressure. Figure 7 shows two calls of the function, having the US units (Fahrenheit degrees and psi – pounds-force per square inch) and European units (Celsius degrees and MPa).

It also has been developed the technique for creating a *function of two arguments* (for example, temperature and pressure) returning thermal physical properties of the substances in *one-phase region*. The technique is described in details in [3]. Its base is spline interpolation of a sparse matrix (table) the

first column of which contains temperature values and the first row pressure does. The remaining part of the matrix contains the calculated values (density, specific entropy, specific enthalpy, etc.)

Conclusion

The described information technology enables us to generate user functions returning properties of the substances quickly and with adequate accuracy.

References

1. A. A. Vasserman, V. P. Malchevskiy, *Databases and automated information systems on thermal physical properties of gases and liquids*// (Technical gases, No. 5, 2009) [in Russian]
http://www.nbuu.gov.ua/Portal/natural/TG/2009_5/2009_5_59-66.pdf
2. A.A. Alexandrov, V.F. Ochkov, K.A. Orlov Steam Tables and Diagrams on Mathcad Calculation Server for Personal Computers, Pocket Computers and Smart Phones // Proceedings of the 15th International Conference of the Property of Water and Steam, Berlin/Germany, September 7–11, 2008 (<http://twf.mpei.ac.ru/ochkov/WSPHB/Berlin2008.pdf>)
3. V. F. Ochkov “Publication of thermal physical properties of the substances: the problems and solutions for the work with tables” Trudy Akademenergo, No 2, 2009 [in Russian]
(<http://twf.mpei.ac.ru/ochkov/TablSite>)