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INSTITUTO DE INGENIERÍA ENERGÉTICA
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Research Publications

CALCULATION OF REFRIGERANT PROPERTIES BY LINEAR INTERPOLATION OF BIDIMENSIONAL MESHES

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ABSTRACT

In order to simulate the behaviour of a thermodynamic system, firstly it is needed to calculate the thermodynamic properties of the system working fluid. In case of refrigeration systems and heat pumps, it is used to refer to the NIST REFPROP database to calculate such properties. The database uses equations of state to calculate the properties of pure refrigerants and refrigerant mixtures. The direct use of the NIST REFPROP database can be problematic due to the high computational time delay, which occurs when it is necessary to solve the equations of state using iterative methods, especially in case of refrigerant mixtures. In the present article is presented a methodology to generate pure refrigerant and refrigerant mixtures properties maps, using a the NIST REFPROP database and its later use by means of interpolation functions, which allows calculations in all the working range, with good precision and speed. The application of the proposed methodology allows generate properties maps for saturated liquid, saturated vapour, subcooled liquid and superheated vapour.

1. INTRODUCTION

In the simulation of thermal systems, one of the first steps is to have a reliable means to calculate the thermodynamic properties of the fluids that circulate around the system. For the case of the refrigeration systems and heat pumps, such calculation of properties are referred always to the NIST REFPROP data base, which uses equations of state for calculating the properties of pure refrigerants and refrigerant mixtures. The direct use of these data bases can be problematic due to the high time consumption when must to solve the equations of state by iterative methods, especially for the case of refrigerant mixtures. Moreover, it has been found by the authors that there is a region around the critical point where such calculation may not produce reasonable results.

Due to both the problems mentioned above, in this paper is proposed a methodology to generate pure refrigerants and refrigerants mixtures properties maps, from the NIST REFPROP v 7.0 database, and its later use by means of interpolation functions, allowing a calculation in all the working range, with good precision and speed.

According to the proposed methodology, properties maps with two degrees of freedom are generated varying the saturation pressure and the subcooled or superheated temperatures. Moreover, properties maps are generated for:

- saturated liquid, varying the saturation pressure;
- saturated vapour, varying the saturation pressure;
- subcooled liquid, varying pressure and temperature;
- subcooled liquid, varying density and temperature;
- superheated vapour, varying pressure and temperature;
- superheated vapour, varying density and temperature.

2. MAPS GENERATION

The maps generation is the result of applying sequentially the following steps:

2.1. Set the constrains of the maps

In this step, the minimum saturation temperature (or pressure), the maximum saturation temperature (or pressure), the minimum subcooled temperature, the maximum superheated temperature, the minimum density and maximum density are established. These limits values define the boundaries of the different maps.

The liquid and vapour saturated lines are limited by the minimum and the maximum saturation temperatures. The boundaries of the subcooled liquid maps are fixed by the minimum subcooled temperature value and the saturated liquid line. Similarly, working in the superheat region, the superheated vapour maps are constrained by the maximum superheated temperature and the saturated vapour line.

The calculation of the limits of the maps proceeds as follow:

a) Calculation of minimum temperature
   The minimum temperature is equal to the maximum of the following values:
   $Tmin_1$ = max ($Tmin_i$), where i is the index of the component for refrigerant mixtures, given in NIST REFPROP function **limitk** for the different options (EOS, ETA, TCX, STN)
   $Tmin_2$ = **limitx** (Tmin), limitx is a function given in NIST Refprop

b) Calculation of maximum temperature and pressure, given by NIST Refprop
   Tmax = **limitx**(T_{max})
   Pmax = **limitx**(P_{max})
   ρ_{max} = **limitx**(ρ_{max})

c) Calculation of critical properties
   T_{crit}, P_{crit}, ρ_{crit}= critical function given in NIST REFPROP

And finally, the limits of the maps are:

Minimum subcooled liquid temperature	:$T_{sc\ min} = T_{min}$
Minimum saturation temperature	:$T_{sat\ min} = T_{sc\ min} + 5.0$
Maximum saturation temperature	:$T_{sat\ max} = 1.1\ T_{critic}$
Maximum superheated vapour temperature	:$T_{sh\ max} = T_{max}$
Maximum density	:ρ_{max}
Minimum density	:$\rho_{min} = \rho sat(T_{sat\ min})$
Maximum pressure	:p_{max}

Also, the ($T_{sc\ min}$, ρ_{max}) , ($T_{sh\ max}$, ρ_{max}) points must to be verified.

2.2. Generate saturated liquid and vapour lines

At this point, the liquid and vapour lines are divided in three zones: sub critical zone, critical point, super critical zone. The sub critical zone is determinate by the minimum saturation temperature (or pressure) and the critical temperature (or pressure), minus a regular value that indicates a band around the critical point. From the calculation point of view the critical point represents a special situation for which can be impossible to obtain property values using the state equations. The super critical zone is the region between the maximum temperature and the critical point plus a regular value that indicates a band around the critical point. The objective of this part is to get the saturated pressure mesh and the properties for each pressure point in bubble and dew conditions for each one of zone mentioned. These calculated properties at saturation will be used to generate the temperature-pressure and temperature-density maps.

a) Sub-critical zone
   The mesh generation process in the sub-critical zone define the saturation properties for bubble and dew point varying the saturation temperature from the minimum saturation temperature found before to the critical point, through regular increases of temperature. In the Fig. 1(a) is shown a scheme of the implemented algorithm

b) Critical point
   From the NIST Refprop routines is obtained the critical values for pressure, temperature and density, so that,

$$\begin{aligned} P_i &= P_{crit} \\ T_i &= T_{crit} \\ \rho_i &= \rho_{crit} \end{aligned} \quad (1)$$

The remainder properties of this point are calculated by a linear extrapolation from of two points above of the critical point, for instance:

$$T_1 = T_{crit} + 3\ K$$
$$T_2 = T_{crit} + 6\ K$$

and, extrapolating

$$\phi_{crit} = \phi_1 - (\phi_1 - \phi_2) * (T_1 - T_{crit}) / (T_1 - T_2) \quad (2)$$

where ϕ_i are the corresponding properties calculated by

$$\phi_i = \phi(T_i, \rho_{crit}) \quad (3)$$

this procedure is used for calculating all properties except surface tension that is null in the critical point.

c) Super critical zone
The mesh generation for super-critical zone define a pseudo-saturation line, where the properties will be calculated, varying the temperature from the maximum temperature found above to the critical point, for a fixed number of point selected. In the Fig. 1(b) is presented a scheme of the implemented algorithm. Through the pseudo-saturation line a constant density equal to the critical density is considerate, with surface tension equal to 0.

2.3. Generate two-dimensional maps

There are two different maps generates, T-p map and T-ρ map. T-p map is generated using lines of constant pressure from de saturation line and from each line the temperature is varied from the saturation temperature to its maximum or minimum value (depending of the region, superheated or subcooled). The T-ρ map is generated in the same way using lines of constant density in this case. The reason of using maps with constant pressure or density will be clarified later.

a) Subcooled liquid temperature-pressure map (SC T-p map)
In this part a two-dimensional mesh is generated varying the temperature between the bubble temperature and the minimum subcooled temperature for each pressure value calculated in the 2.2. section. A scheme of the algorithm implemented is shown in the Fig. 1(c). For this case the X variable in the Fig. 1(c) indicates the corresponding pressure.

b) Superheated vapour temperature-pressure map (SH T-p map)
A two dimensional mesh is generated considering a constant pressure determinate by each saturated pressure calculated in 2.2. and varying the temperature between the dew temperature and the maximum superheated temperature. The algorithm scheme is shown in the Fig 1(d). Again, the X parameter in the Fig. 1(d) indicates the corresponding pressure.

c) Superheated Vapour density-temperature (SH T-ρ map)
A two dimensional mesh is generated considering a constant saturation density value determinate by each saturated pressure calculated in 2.2., varying the temperature between the saturated temperature and the maximum superheated temperature. The algorithm scheme is shown in the Fig 1(d). Like to the SH T-p map, the X parameter in the Fig. 1(d) indicates the corresponding density.

d) Subcooled liquid density-temperature map (SC T-ρ map)
A two dimensional mesh is generated considering a constant saturation density value determinate by each saturated pressure calculated in 2.2., varying the temperature between the saturated temperature and the

minimum subcooled temperature. A scheme of the algorithm implemented is shown in the Fig. 1(c). For this case the X parameter in the Fig. 1(c) indicates the corresponding density.

3.0. Interpolation

Once the maps are generated, the calculation of the refrigerant properties consists of making a one-dimensional linear interpolation through the saturated lines and a bilinear interpolation for points in the subcooled or superheated region.

3.1. Saturated liquid and vapour lines.
The interpolation for the saturated lines can be made using either saturated temperature or pressure and it depends on the bubble or the dew point.
The first step to take now is to find the values range where the actual pressure (or temperature) is located, and which represents a constraint to the interpolation. After, the non-dimensional parameter ε is calculated by the following expression:

$$\varepsilon = (X - X_1)/(X_2 - X_1) \tag{4}$$

where X_i is the pressure o temperature of the i_{th} node, and X and the pressure or temperature known.

Moreover, the remainder properties are calculated by using the equation:

$$\phi = \phi_1 + \varepsilon * (\phi_2 - \phi_1) \tag{5}$$

where ϕ_i is property that corresponds to the i_{th} node.

3.1. Subcooled liquid and superheated vapour maps
For T-p and T-ρ maps, a bilinear interpolation is implemented, which allows to calculate values for the following pair properties: pressure and temperature, pressure and enthalpy, pressure and entropy, temperature and density. As done for the saturated lines, the procedure starts searching the corresponding region where the couple of known properties is located. Once the region is found, the region is mapped to a normalized system where the interpolation will be executed. Finally, the calculated properties in the normalized system are mapped back to the original system, as is shown in the Fig. 2.

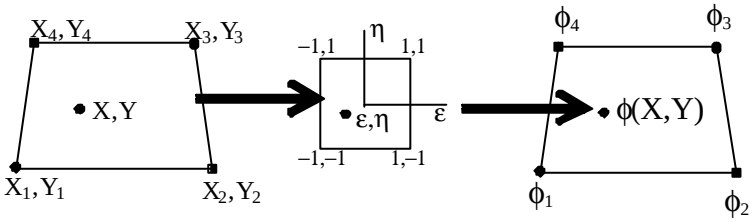

Figure 1. Interpolation method

In general, the interpolation method assumes that the properties can be calculated using linear shape functions N_i defined in the (ε,η) space of the normalized element:

$$\Phi = \sum [\Phi_i * N_i(\varepsilon, \eta)] \tag{6}$$

where Φ_i are the properties at the four nodes of the element.

N_i are the shape functions for the normalized element, defined as

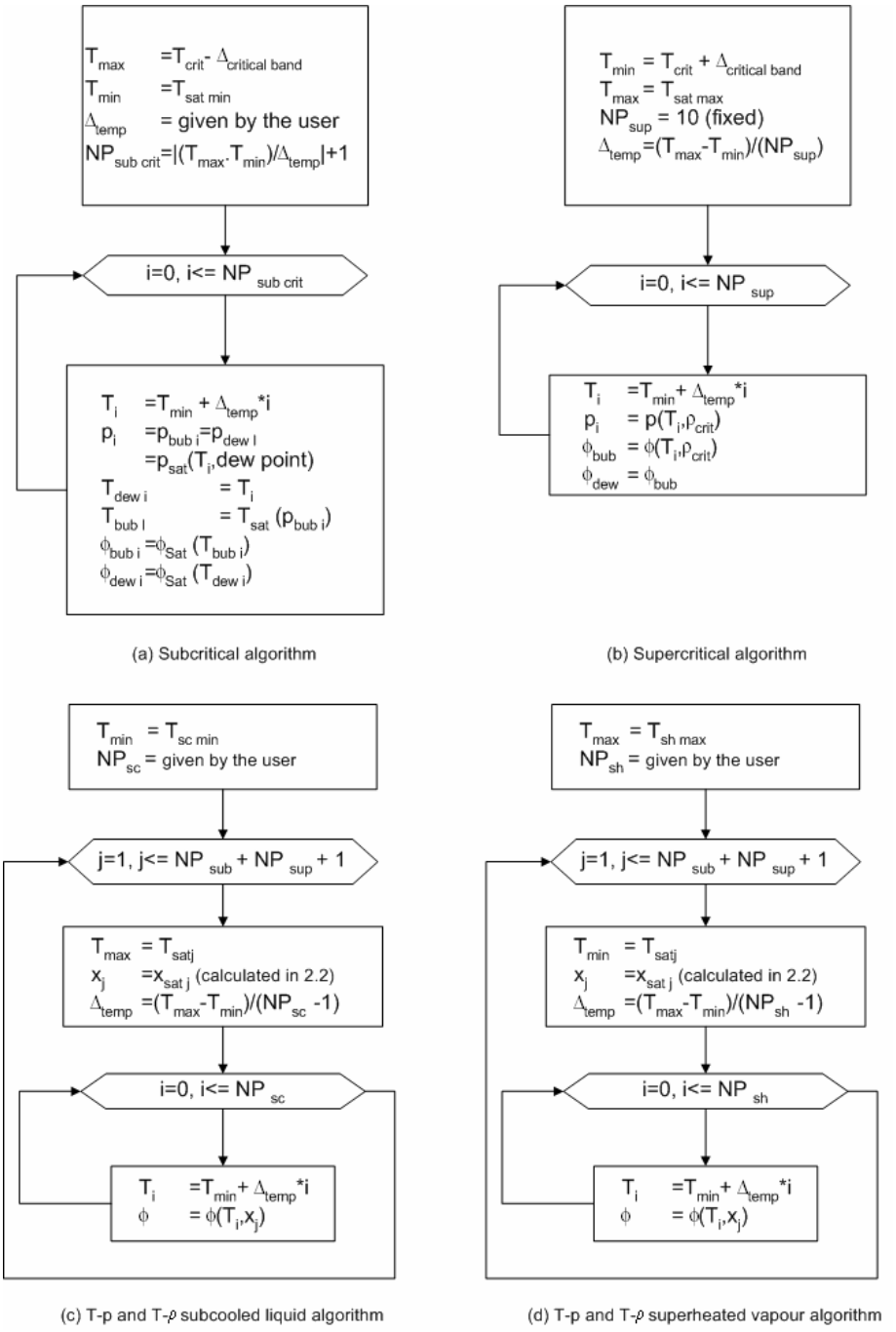

Figure 2. Flow charts for the different options of maps generation

$$N_1 = \frac{(1-\varepsilon)(1-\eta)}{4} \qquad N_2 = \frac{(1+\varepsilon)(1-\eta)}{4}$$
$$N_3 = \frac{(1+\varepsilon)(1+\eta)}{4} \qquad N_4 = \frac{(1-\varepsilon)(1+\eta)}{4} \tag{7}$$

The mapping of the (X,Y) plane into (ε,η) is given by the following equations

$$X = \sum \left[X_i * N_i(\varepsilon,\eta) \right] \tag{8.a}$$

$$Y = \sum \left[Y_i * N_i(\varepsilon,\eta) \right] \tag{8.b}$$

In general, is not possible to give an explicit equation in the form of $\varepsilon=f(X,Y)$ and $\eta=f(X,Y)$, which forces to solve a system of equation for each pair of (X,Y) .

For the particular case that $Y_1=Y_2$ and $Y_3=Y_4$ (the quadrilateral is a parallelogram), we can find and explicit solution of the form:

$$\varepsilon = \frac{(X_1 - X_2)*Y + (Y_2 - Y_1)*X + X_2*Y_1 - X_1*Y_2}{(X_1 - X_2 + X_3 - X_4)*Y + (X_2 - X_3)*Y_1 + (X_4 - X_1)*Y_2} \tag{9}$$

$$\eta = \frac{(Y - Y_1)}{(Y_3 - Y_1)} \tag{10}$$

where Xi, Yi are the known properties at the mesh nodes. This is the reason why the maps are generated using lines of constant pressure or density, that is, the mesh is formed by parallelograms.

Then, the procedure of calculating a thermophysical property Φ given two independent properties X and Y, is first calculate ε and η and from de Equations 9 and 10, and then using the shape functions from Equations 7 to obtain the interpolated property from the values a the nodes of the mesh Φ_i.

4. RESULTS

The Figure 3 shows a typical generated map in a pressure-enthalpy diagram. In order to see how are the different maps, the maps are generated with few nodes. The horizontal lines in the part (a) corresponds to the constant pressure lines mentioned before, is clearly shown how the parallelogram is formed between constant pressure lines and constant temperature lines. In the same way, in part (b) is shown the corresponding parallelograms for the temperature-density maps. Now the parallelograms are rotated and the shape function can be applied without problem. Moreover, in both cases, it can be observed how clear the profile of the saturated lines is .

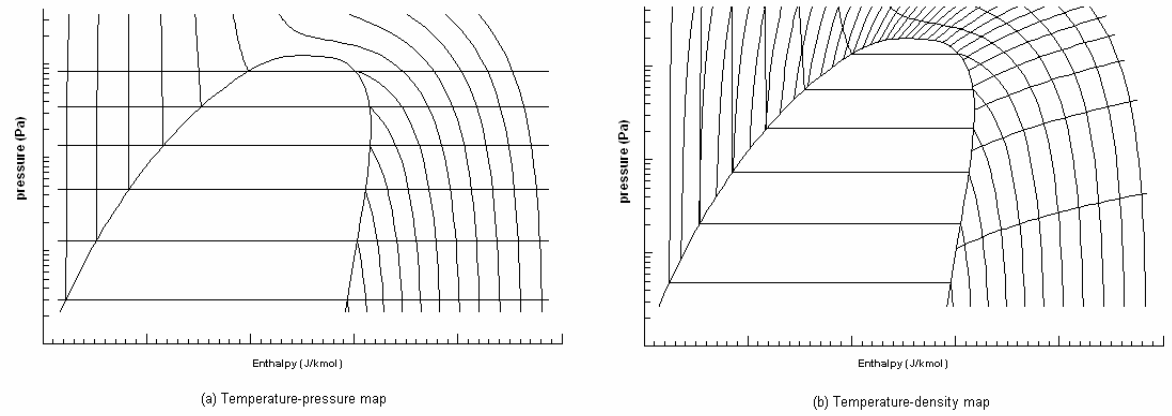

Figure 3. Pressure-enthalpy diagram for the generated maps. (a) Temperature-pressure map, (b) Temperature-density map

In order to estimate the effectiveness of the procedure implemented, the following tests were taken:

1) For each refrigerant in NIST Refprop database, more than 1000 properties points were calculated, including:
   - Points for saturated liquid and vapour pressures and temperatures,

- Points for subcooled liquid and superheated vapour for: pressures and temperatures, pressure-enthalpy, pressure-entropy, temperature-density known.

The accuracy of the interpolation method is determinate comparing with the calculations results using the NIST Refprop routines. Table 1 shows the definitions of the average, maximum and standard deviation between the values calculated by interpolation routines (subscript "int") and the values calculated by NIST ("NIST" subscript). The deviations obtained between the properties calculated using the interpolation method and using the NIST Refprop routines are shown in the Table 2. Here, are shown deviations for some common refrigerants: R22, R134a, R407C and R410A. Moreover, only the properties with the higher error values are visualized. As can be observed, the interpolation method gives a high accuracy, with maximum errors less than 1% for the most of properties. For Cp, for all refrigerants analyzed, the high maximum error was found in points close critical point, and this occurrence explains the obtained values for the average and standard deviation. A solution for this high error could be to obtain the properties of the critical point from points located closer than the critical point.

2) The computational time delay to calculate 1000 points in subcooled and superheated region for R22, R134A, R407C, R410A refrigerants, using the interpolation maps, was calculated; the results are compared with the time delay related to the use of the NIST Reprop database as is shown in the Table 3. It is useful to notice that, in all cases, the time delay using the interpolation routines was smaller than that using the NIST Reprop and, in mixtures cases, the time delay was even smaller.

Table 1. Definition of statistical number to evaluate the predictive accuracy of interpolation method

Deviation	Av. Deviation	Max. Deviation	Std. Deviation
$E_i = \frac{\phi_{int} - \phi_{NIST}}{\phi_{NIST}} * 100$	$E_{AV} = \frac{\sum E_i}{NP}$	$E_{MAX} = \max(E_i)$	$E_{STD} = \frac{\sum (E_i - E_{AV})}{(NP-1)}$

Table 2. Comparison of the calculated properties using the interpolation method respect to the properties calculated using NIST Refprop routine

Ref.	Property														
	Enthapy			Entropy			Cv			Cp			Density		
	Av. Dev. (%)	Max. Dev. (%)	Std dev. (%)	Av. Dev. (%)	Max Dev. (%)	Std Dev. (%)	Av. Dev. (%)	Max. Dev. (%)	Std. Dev. (%)	Av. Dev. (%)	Max. Dev. (%)	Std. Dev. (%)	Av. Dev. (%)	Max. Dev. (%)	Std. Dev (%)
R22	0.004	0.159	0.012	0.002	0.096	0.01	-0.008	0.346	0.023	-0.076	6.18	0.42	0.003	0.528	0.045
R134a	-0.005	0.268	0.017	0.002	0.168	0.013	-0.01	0.841	0.049	-0.101	13.54	0.742	0.007	1.695	0.091
R407C	-0.005	0.142	0.011	0.002	0.088	0.009	-0.007	0.416	0.025	-0.054	4.201	0.244	0.004	0.47	0.038
R410A	-0.005	0.25	0.017	0.001	0.164	0.013	-0.014	0.796	0.052	-0.092	9.992	0.524	0.005	0.756	0.056

Table 3. Time consumption for calculating 1000 points using NIST Refprop routines and the proposed interpolation method

Time (seg)	Refrigerant			
	R22	**R134A**	**R407C**	**R410A**
NIST	2.59	1.54	45.31	23.12
Interpolation	0.05	0.05	0.06	0.06

5. CONCLUSIONS

A methodology to generate refrigerant maps and their later use in the calculation of properties was managed to develop and to validated. The resulting error, respect to the NIST Refprop routine is smaller than 1%. In the supercritical region, in the vicinity of the critical point, the error for the calculation of Cp is greater due to the asymptotic behaviour that presents the real calculation of the Cp property, and for the interpolation method the properties on critical point was obtained in an approximate form. The proposed method allows calculating the properties of refrigerant in all range within the limits of the maps. Finally, a considerable reduction of calculation time is obtained, especially for refrigerant mixtures, when the interpolation method is used.

6. ACKNOWLEDGEMENTS

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NOMENCLATURE

p	Pressure, Pa
T	Temperature, K
ϕ,Φ	indicates any thermophysical or transport property ($h,s,C_p,C_v,\rho,\mu,k,\sigma,\ldots$)
H	enthalpy, J/kmol
ρ	density, kmol/m^3
s	entropy, J/kmol K
C_p	specific heat at constant pressure, J/kmol K
C_v	specific heat at constant volume, J/kmol K
μ	viscosity, Pa s
k	thermal conductivity,
σ	superficial tension, N m
η	non-dimensional factor
ε	non-dimensional factor
N	interpolation function

Subscripts:

AV	average
crit	critical point
NIST	NIST Refprop database
max	Maximum
min	Minimum
sat	saturated
sh	superheated
sc	subcooled
sh	superheated
temp	temperature
dew	dew point
bub	bubble point

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