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A USER-FRIENDLY SOFTWARE FOR COMPUTATIONS OF VAPOR COMPRESSION CYCLES WITH PURE FLUIDS AND ZEOTROPIC MIXTURES

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ABSTRACT

The purpose of this paper is to present how models for the computation of thermodynamic and transport properties have been used in a microcomputer program, in a user-friendly Windows® environment, specially designed to help solving refrigeration and air conditioning engineering problems.

In a first part the basic equations and computation methods for pure fluids and zeotropic mixtures are presented.

In a second part we present the general structure and the main characteristics of the program:

- edition of tables for saturated and superheated refrigerants.
- exhaustive study of one-stage or two-stage vapor compression cycles.
- cycle comparisons with different refrigerants

INTRODUCTION

Six years ago, we presented here a paper describing a new software which allowed their users to make easy computations on one-stage and two-stage vapor compression cycles and useful comparisons for different type of cycles or refrigerants. Five hundred packages of this software have been sold until now, mainly for educational purpose.

The software was intended to be used in a DOS environment and applied only to pure refrigerants and their azeotropic mixtures including CFC's, HCFC's, Ammonia and later HFC's.

The new version presented now, is developed in a Windows® environment in order to follow the considerable evolution of the computer technics and computation speedness.

This version includes also some zeotropic mixtures of HCFC's and HFC's refrigerants.

As previously, the new version is intended to help Refrigeration and Air Conditioning people in solving engineering and servicing problems.

BASIC EQUATIONS

Vapor Pressure

For pure refrigerants and azeotropic mixtures, the same law with one set of coefficients applies to the bubble and dew points; for zeotropic mixtures, on contrary, two different sets of coefficients are to be used.

The vapor pressure correlation is implemented in the form:

$$\ln P = \sum_{i=1}^9 a_i T^{-2} + (a_{10} + a_{11} T) \ln T + (a_{12} / T + a_{13}) \ln(a_{14} - T) + a_{15} T^{14} + (a_{16} / T + a_{17}) (a_{18} - T)^{3/2}$$

Liquid Density

The liquid density, based on the corresponding state method, may be written as follows:

$$\rho' = b_0 + \sum_{i=1}^9 b_i (1 - T_r)^{i/3} + b_{10} (1 - T_r)^{1/2} + b_{11} (1 - T_r)^{3/2}$$

T_r being the reduced temperature.

Heat Capacity

In the vapor phase, the heat capacity is conveniently represented through the ideal gas state heat capacity which is correlated from experimental data in a polynomial form:

$$C_v^0 = \sum_{i=0}^{11} c_i T^{i-5}$$

The constant volume heat capacity is obtained from this equation by integrating at constant temperature:

$$C_v = C_v^0 + T \int_{\infty}^v \left(\frac{\partial^2 P}{\partial T^2} \right)_v dV$$

The constant pressure heat capacity is also computed by:

$$C_p = C_v - T \frac{\left(\frac{\partial P}{\partial T} \right)_v^2}{\left(\frac{\partial P}{\partial v} \right)_T}$$

Equation of State

For most of the pure refrigerants and azeotropic mixtures, the Martin Hou equation of state is used except for ammonia (Morsy) and R13b1 (Rombush).

For zeotropic mixtures a cubic equation of state has been chosen:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)} \quad \text{or also} \quad Z^3 - Z^2 + Z(A-B-B^2) = 0$$

$$Z = \frac{PV}{RT} \quad A = \frac{aP}{R^2 T^2} \quad B = \frac{bP}{RT}$$

where b is defined as : $b = \sum_i X_i b_i$ with $b_i = 0.08664 \frac{RT_{ci}}{P_{ci}}$

and a is temperature dependent coefficient : $a = \sum_i \sum_j X_i X_j (a_i a_j)^{0.5} (1 - k_{ij})$

with $a_i = a_{ci} \left(1 + m_i (1 - T_r^{0.5}) - p_i (1 - T_r) (0.7 - T_r) \right)^2$ where $a_{ci} = 0.42747 \frac{R^2 T_{ci}^2}{P_{ci}}$

and $m_i = 0.48508 + 1.55191 \omega_i - 0.15613 \omega_i^2$

For each i component : T_r reduced temperature, T_{ci} P_{ci} critical values, ω_i acentric factor.

THERMODYNAMIC PROPERTIES

Vapor-liquid Equilibria

For zeotropic mixtures, the vapor-liquid equilibria may be calculated from the condition:

$$\frac{\Phi_i^L}{\Phi_i^V} = \frac{Y_i}{X_i} \quad \text{where } Y_i \text{ is the vapor mole fraction of component } i, X_i \text{ is the liquid}$$

mole fraction of the same component and Φ_i its fugacity coefficient.

Density and Mass Volume

In the vapor state, from T and P the mass volume or the density may be calculated with the help of the state equation; in case of zeotropic mixtures, the resolution of the cubic equation of state gives the larger root Z_v then $V_v = Z_v \frac{RT}{P}$

The larger root Z_v and the lower root Z_L are also used for enthalpy and entropy calculations.

In the liquid state, the density (and the mass volume) is calculated as previously shown.

Enthalpy and Entropy

Enthalpy is obtained from the thermodynamic relationship:

$$dh = C_v dT + \left[T \left(\frac{\partial P}{\partial T} \right)_v - P \right] dV + d(PV)$$

In the same way entropy is obtained from:

$$ds = \frac{C_v}{T} dT + \left(\frac{\partial P}{\partial T} \right)_v dV$$

The constant volume heat capacity is calculated as previously shown and $\left(\frac{\partial P}{\partial T} \right)_v$ calculated from the equation of state.

Heat of Vaporization

For pure fluid the heat of vaporization is given by the Clapeyron equation:

$$L = 100T \frac{dP}{dT} (V_v - V_L)$$

where $\frac{dP}{dT}$ is obtained by the vapor pressure equation derivative and V_v and V_L are the mass volumes in vapor phase and in liquid phase respectively at the same pressure.

For zeotropic mixtures the heat of vaporization is calculated by the difference of enthalpy in vapor phase and enthalpy in liquid phase at constant pressure using the roots Z_v and Z_L of the cubic equation of state.

NUMERICAL SUBROUTINES

Subroutines

A complete set of subroutines is included in the program in order to solve the basic equations described in the preceding sections.

When modeling a refrigeration or air conditioning cycle, the direct computation of these equations with direct inputs is generally not sufficient and it is typically necessary to use mathematical tools to solve them in a reverse way.

For example the equation for the vapor pressure may be solved as $P = f(T)$ but $T = f(P)$ may be requested as well.

The process in the expansion valve may be considered as isenthalpic or in some cases as isentropic and the user need to have the complete set of thermodynamic properties with the temperature or pressure and enthalpy or entropy as inputs in the two-phase area.

In the same way the thermodynamic properties of the refrigerant at the end of the compression have to be computed taking in account the isentropic efficiency of the compressor and these properties must be calculated also with temperature or pressure and enthalpy or entropy as inputs in the vapor area.

Numerical Tools

The numerical tools typically used are :

- Dichotomy
- Secant method
- Newton's method
- eventually other iterative technics

In order to insure speedness, accuracy and reliability of computations it is necessary to make a proper choice of the method(s) used, of the convergence criterion and a strict control of the convergence. Each particular calculation has been tested using different algorithms and systematic comparisons between them have been done.

Particular Cases

In the cycle simulations, mainly with zeotropic mixtures, it may be necessary to calculate the thermodynamic properties of a particular point of the cycle in relation with other points.

For example the condensing temperature may be known as mean condensing temperature and must be related to the corresponding dew and bubble points at same pressure, if no pressure drop is involved; but the same point, in the two-phase area, must also been calculated individually, if requested, with temperature and pressure as inputs.

This applies also for the mean evaporating temperature and the corresponding point which may be related to the preceding and the following points or studied individually.

TRANSPORT PROPERTIES

The transport properties, dynamic viscosities and thermal conductivities, are mainly computed with the help of the compilation of experimental data and predictive methods from D. Jung and R. Rademacher (ASHRAE Transactions).

SOFTWARE PACKAGE

The complete software has been written for use in a Windows® environment and follows the general requirements of this environment. The numerical core has been implemented in Turbo Pascal libraries which may be used for other programs.

The main possibilities included are:

- Choice of units: SI, US or technical.
- The reference point for enthalpy and entropy calculations may be chosen also.
- Choice of refrigerant: 20 pure or azeotropic fluids, 4 zeotropic mixtures.
- Thermodynamic and transport properties of a single point of a system in liquid, vapor or two-phase area.
- Complete cycle modelisation for one stage, two-stage or cascade systems.
- Energy and capacity analysis with comparisons between different cycles or fluids.

The cycle modelisations are done on a spreadsheet, each line, fully documented, corresponding to a particular point of the system studied. When the necessary input(s) are entered the remaining properties are calculated. If more than one point is related to this or these inputs the properties of the other related points are also computed (if requested by the user).

The complete cycle may be displayed on the Mollier diagram of the refrigerant and printed as well by a laser or ink bubble jet printer.

As required, the cycle modelisation, energy and capacity analysis may be printed by the printer and may be saved on the hard disk and retrieved from it.

CONCLUSION

The software briefly presented here is a complete remodeling of the previous version including some zeotropic mixtures and a completely new environment and design.

The International regulations restricting the production of HCFC's after the complete ban of CFC's involve the development of the technical knowledge in the Refrigeration and Air Conditioning field, this software has been designed as a support to meet this requirement.

NOMENCLATURE	
C : heat capacity	<i>subscripts:</i>
h : enthalpy	c: critical values
L : latent heat	i, j: component #
P : absolute pressure	L: liquid
R : gas constant	V: vapor
s : entropy	
T : temperature	<i>superscripts:</i>
V : mass volume	°: ideal gas state
X : liquid mole fraction	' : liquid state
Y : vapor mole fraction	
Z : compressibility factor	
Φ : fugacity coefficient	
ρ : density	

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