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A COMPUTER SOFTWARE FOR THERMODYNAMIC PROPERTIES COMPUTATION AND REFRIGERATION SYSTEMS DESIGN

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ABSTRACT

The aim of this paper is to present how models for computation of thermodynamic properties have been used to develop a reliable and easy-to-use microcomputer program, specially designed to help in solving refrigeration engineering problems.

The first part of the paper is devoted to the presentation of basic equations and numerical methods which constitute the core of the program.

In the second part we present the general structure and main capabilities of the software developed at L.T.I.. Among the main options are :

- automatic editing of tables for superheated vapor or saturated liquid vapor state ;
- possibility to define a thermodynamic cycle by any set of valid data (T,P,H,S) and to perform exhaustive analysis of a corresponding machine.

INTRODUCTION

Although accurate models for computation of thermodynamic properties for most refrigerant fluids have been available for some time, until now they have only been used in industry through the channel of various tables and charts.

The widespread use of microcomputers and their increasing computational power make it possible now to develop software tools specifically for the refrigeration industry. Thermofluid[®] is such a tool.

Thermofluid[®] is based on a research tool developed at L.T.I. Créteil by researchers working in two different domains: diphasic flow through safety valves and refrigeration systems modelisation. This research tool consists of two main parts:

- a data bank for fluid properties: this data bank consists of four basic equations, together with the coefficients characteristic of each fluid;
- a numerical core, with functions to compute all thermodynamic properties from any set of valid data (for instance, (T,P) or (T,S) in the vapor phase).

As such, and with a simple user interface, this tool has been used successfully both in a research and in an educational context.

Thermofluid[®] is a program based on this research tool, which provides much more sophisticated possibilities and a user-friendly interface; it replaces completely thermodynamic tables and charts, and simplifies the task for analysis of refrigeration systems.

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** Société DEHON SERVICE. France. THERMOFLUID is a DEHON SERVICE property.

I. BASIC EQUATIONS

I.1. EQUATION OF STATE :

The equation of state is mostly given as a relation $P=f(V,T)$ for the vapor phase; this is a semi-empirical equation, which means that the general form is derived from theoretical considerations, but various corrective terms have generally been added. Notice that, this equation being explicit in the variable P , an easy access to partial derivatives such as $(\frac{\partial P}{\partial T})_V$ or $(\frac{\partial P}{\partial V})_T$ is possible.

The data available for refrigerant fluids in the litterature have prompted us to implement three different forms for the equation of state :

1)- Martin-Hou equation is a virial equation of state available for a wide range of fluids (R11, R12, R13, R14, R22, R23, R114, R142b, R152a, R500, R502 and R134a). (EKROTH [1], MARTIN-HOU [2] and WILSON-BASU [4]).

$$P = \frac{r T}{(V-b)} + \sum_{i=1}^5 \frac{A_i + B_i T + C_i e^{-k \frac{T}{T_c}}}{(V-b)^i} + \frac{A_6 + B_6 T + C_6 e^{-k \frac{T}{T_c}}}{e^{a V} (1 + c e^{a V})}$$

2)- Benedict-Webb-Rubin equation has been used in two different modified forms : MORSY [3] (Refrigerant R12b1, R113, R115 and R717) or Mc LINDEN et al. [8] for R123 :

$$\begin{aligned} \frac{P}{P_c} = W_a \sigma \delta + (A_1 + A_2 \sigma + \frac{A_3}{\sigma^2} + \frac{A_4}{\sigma^4}) \delta^2 + (A_5 + A_6 \sigma + \frac{A_7}{\sigma^2}) \delta^3 \\ + (\frac{A_8}{\sigma^2} + \frac{A_9}{\sigma^4}) \delta^3 (1 + \beta \delta^2) e^{-\beta \delta^2} + A_{10} \delta^6 \end{aligned}$$

3)- ROMBUSCH formulation [5] is a corresponding-states equation used for R13b1 :

$$\begin{aligned} \frac{P}{P_c} = 1 - (1 - \delta)^5 [1 + A_0 \delta + \frac{A_1 (A_2 - \delta) \delta^2}{1 + 4 (1 - \delta)^2}] + (\sigma - 1) \sum_{i=1}^6 B_i \delta^i \\ + \frac{(\sigma - 1)^2}{\sigma} \sum_{i=2}^4 C_i \delta^i \end{aligned}$$

I.2. VAPOR PRESSURE :

This is a correlation between temperature and pressure at equilibrium between vapor and liquid phases. It is also very important as it gives the enthalpy of vaporization without need for a distinct correlation. The vapor-pressure correlation is implemented in the form :

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

I.3. LIQUID DENSITY :

Liquid density correlation appears as an extension of Yen and Woods formula, based on the corresponding states method :

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

I.4. IDEAL GAS HEAT CAPACITY :

The heat capacity in the vapor phase is more conveniently represented through the heat capacity C_v^0 in the ideal gas state, which is also the real gas state for very low densities; as is well known, C_v^0 depends on the temperature only and can then easily be correlated either from experimental data or from theoretical data computed from spectroscopic data.

In our data bank, the following general correlation has been implemented:

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

II. COMPUTATION OF THERMODYNAMIC PROPERTIES

All thermodynamic properties in the vapor phase at a given temperature and volume are easily computed from the basic equations above.

II.1. CONSTANT VOLUME HEAT CAPACITY :

$C_v (V,T)$ is obtained from $C_v^0 (T)$ by integrating at constant temperature :

$$C_v (V,T) = C_v^0 (T) + T \int_{\infty}^v \left(\frac{\partial^2 p}{\partial T^2} \right)_V dV$$

II.2. CONSTANT PRESSURE HEAT CAPACITY :

$C_p (V,T)$ is computed by application of Mayer's generalized law :

$$C_p (V,T) = C_v (V,T) + T \frac{\left[\left(\frac{\partial p}{\partial T} \right)_V \right]^2}{\left(\frac{\partial p}{\partial V} \right)_T}$$

II.3. SPECIFIC ENTHALPY :

$H (V,T)$ is obtained by integrating from a reference state H_{ref} first on an isovolumic path and then on an isothermal path :

$$H (V,T) = H_{ref} + \int_{T_{ref}}^T \left[C_v^0 (T) + T \int_{\infty}^{V_{ref}} \left(\frac{\partial^2 p}{\partial T^2} \right)_V dV \right] dT \\ + \int_{V_{ref}}^V \left[T \left(\frac{\partial p}{\partial T} \right)_V - p \right]_T dV + pV - p_{ref} V_{ref}$$

II.4. SPECIFIC ENTROPY :

$S (V,T)$ is obtained in a similar fashion to $H (V,T)$:

$$S (V,T) = S_{ref} + \int_{T_{ref}}^T \left[\frac{C_v^0 (T)}{T} + \int_{\infty}^{V_{ref}} \left(\frac{\partial^2 p}{\partial T^2} \right)_V dV \right] dT + \int_{V_{ref}}^V \left[\left(\frac{\partial p}{\partial T} \right)_V \right]_T dV$$

It should be noticed that all four equations above give rise to analytical expressions for C_v , C_p , H and S , provided that integral terms can be computed.

II.5. ENTHALPY OF VAPORIZATION :

Clapeyron equation gives :

$$L_V = T \frac{dp_s(T)}{dT} (V'' - V')$$

This equation requires the knowledge of $V(P,T)$ and is then the only non-explicit thermodynamic property as a function of (V,T) .

II. NUMERICAL CORE

The first task of the numerical core is of course to compute the four equations above; but it is also to provide a complete set of thermodynamic calculations.

It is often needed to determine some thermodynamic quantities from some known quantities which are not necessarily pressure and temperature. For instance :

- a compressor is often characterized by its isentropic efficiency, which enables the calculation of exhaust enthalpy from inlet conditions: thermodynamic quantities have then to be computed from P and H ;
- the evolution of a fluid flowing through an expansion valve is often considered to be isenthalpic ; enthalpy is thus one of the two quantities from which thermodynamic quantities at the valve exhaust will be computed, the fluid being here in a diphasic state.

All these calculations typically necessitate an inversion of the basic equations (for instance, calculation of $V=V(P,T)$ whereas only $P=P(V,T)$ is directly available). This kind of inversion can be performed by iterative schemes, among which:

- dichotomy ;
- secant method ;
- Newton method.

are the best known.

Newton method is the one of highest convergence speed, but necessitates the knowledge of the first derivative and does not necessarily converge. The secant method is often nearly as efficient but does not use the first derivative. The dichotomy method is much less efficient but convergence is guaranteed.

The qualities required of the functions in our numerical core are:

- fastness ;
- accuracy ;
- reliability.

Reliability is achieved through a mixed use of all three numerical methods above and a strict control of convergence. Fastness and accuracy were obtained through a very strict optimization work and systematic comparison of different algorithms for each particular calculation. Some cases, as computation from given enthalpy and entropy, necessitated the elaboration of a specific original iterative scheme.

All this optimization work proved very useful when developing a general purpose software such as Thermofluid[®], as it is well known that a response time of more than one second always seems painfully long to the user; accuracy and reliability are of course even more important.

III. THE THERMOFLUID[®] SOFTWARE

The overall structure of Thermofluid[®] is illustrated on Fig. 1.

The main possibilities offered are :

- choice of units ;
- choice of refrigerant fluid ;
- thermodynamic characteristics for a given point ;
- editing of user-defined tables for superheated vapor or saturated liquid/vapor state ;
- Cycle/Machine analysis.

We shall describe here only the last function, as it is the most complex.

The Cycle Analysis module offers the user a spreadsheet-like table (Fig.3) in which he can enter the information he has about the different points of the cycle; the remaining characteristic properties are automatically computed as soon as the information is sufficient. The spreadsheet format is automatically provided by the choice of a cycle type (Fig. 2); this type can be selected among three predefined types ;

- A : single-stage ;
- B : two-stage partial injection ;
- C : two-stage total injection.

User-defined types are also available through option D. ; the user then defines the domain (vapor, liquid etc.) of each point and can save this definition for later use.

The cycle can be visualized at any stage on a Mollier diagram; also available is the edition of complete characteristics (including for instance viscosity or conductivity) for any point in the cycle.

Error checking can be enforced and will then provides error messages whenever some impossibility occurs in the cycle definition, such as compressor exhaust pressure inferior to the inlet pressure.

Once all the points essential to the definition of the cycle have been entered, the analysis of the cycle becomes available ; at this point, it is also possible to define a machine operating on this cycle and to perform a complete analysis of this machine (Fig.4).

Lastly, different machines operating on the same cycle can be edited together for ready comparison of performances : for instance, the engineering consequences of replacing the existing fluid in a machine by a new substitute can thus be investigated with a minimal amount of work (Fig.5).

Many additional facilities are of course available at any moment :

- saving and retrieving on disk at any stage of the work ;
- SI, Technical and US units, with automatic conversion of entered data and possibility to mix and to switch between systems ;
- edition on printer of cycle or machine definition and analysis ;
- edition on plotter of Mollier diagram and cycle.

CONCLUSION

It has been said that to face the new regulations now emerging in all advanced countries, the refrigeration industry will have to develop its technical ability and performances ; we hope that such a tool as we have presented can help in this evolution.

This tool is the product of a continued collaboration between research workers and refrigeration systems specialists ([6]-[7]); this kind of collaboration should help it evolve to meet future industrial needs.

Among the possible additions is the possibility to work with complex mixtures of fluids; another interesting enhancement would be the development of an expert system interface to help the user in his choices.

NOMENCLATURE	
H : specific enthalpy	C_v : specific heat at constant volume
M : molar mass	C_p : specific heat at constant pressure
P : absolute pressure	L_v : latent heat of vaporization
R : perfect gas constant	<i>Greek letters :</i>
r = R/M	ρ : density
S : specific entropy	δ = V _c /V
T : temperature	σ = T _c /T
V : specific volume	<i>Superscripts :</i>
<i>Subscripts :</i>	° : ideal gas state
c : thermodynamic critical point	" : saturated vapor state
s : saturated	' : saturated liquid state

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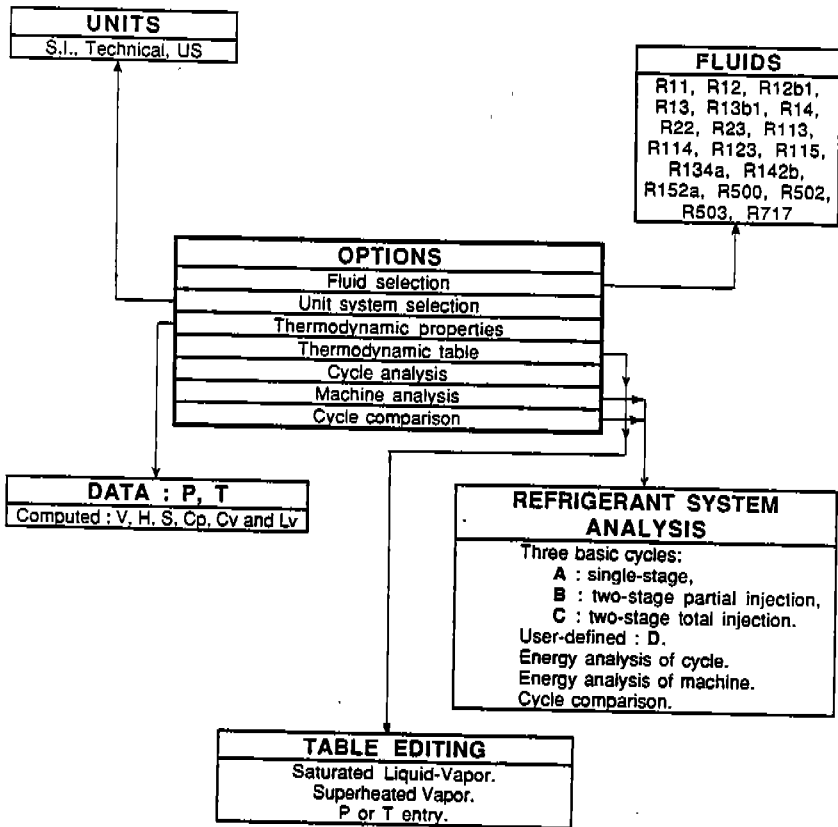


Fig. 1 : Program structure.

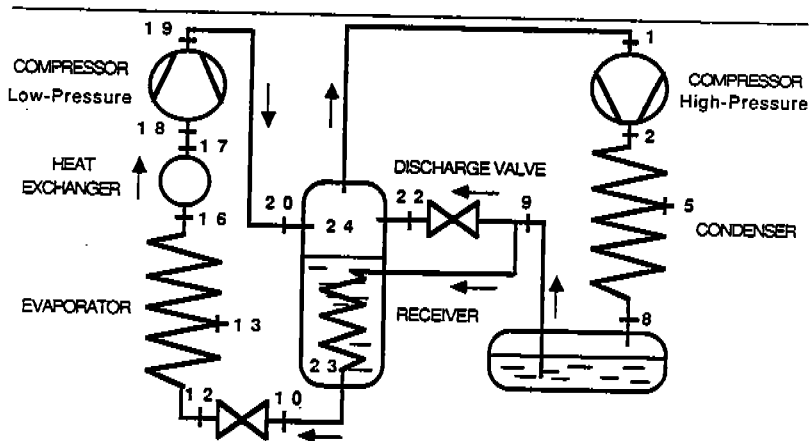
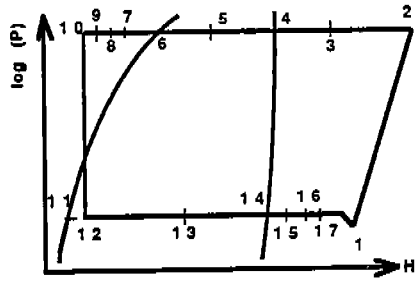
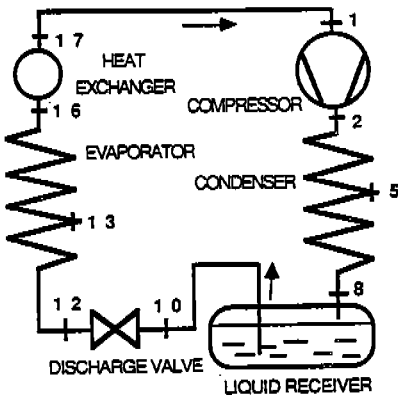
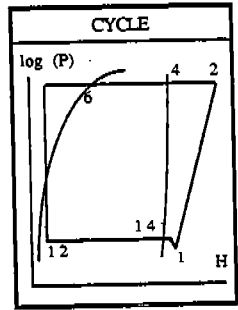


Fig. 2 : Cycle B : two-stage partial injection.



No	T °C	P bar abs	H kJ/kg	S kJ/kg.K	Xvap %
1	-25.00	0.95	341.13	1.5909	superheated
2	54.15	7.65	380.93	1.5969	superheated
3	superheated
4	30.00	7.45	363.58	1.5434	sat. vap.
5
6	28.71	7.20	227.29	1.0939	sat. liq.
7	subcooled
8	subcooled
9	subcooled
10	20.00	7.02	218.85	1.0656	subcooled
11	-27.84	1.10	174.71	0.9029	sat. liq.
12	-28.95	1.05	218.85	1.0837	0.27
13
14	-30.00	1.00	338.10	1.5750	sat. vap.
15	superheated
16	superheated
17	superheated

File : MachineA
 Fluid : R12
 Cycle : A
 Dir : C:\



CURRENT POINT

Compressor inlet
 Essential point
 Completely defined

HELP

<ARROWS> : Move about
 <RETURN> : Validate
 <ESC> : Abort operation
 <F9> : Print spreadsheet
 <F7> : Cancel line

F1 : CYCLES F2 : UNITS F3 : FACILITIES F4 : ANALYSIS F10 : QUIT

Fig. 3 : Example : cycle A. Using spreadsheet.

ENERGY ANALYSIS OF MACHINE

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Fluide : R12
Cycle : A
File : MachineA

Compressor exhaust pressure	bar abs	7.65
Condenser inlet temperature	°C	30.00
Compressor inlet pressure	bar abs	0.95
Evaporating temperature	°C	-30.00
Compression ratio	ratio	8.05
Volumetric production at condenser	kJ/m3	888.62
Volumetric production at evaporator	kJ/m3	689.75
Volumetric work of compressor	kJ/m3	230.18
Compressor exhaust temperature	°C	54.15
Condensing power	kW	6.44
Evaporating power	kW	5.00
Mass flow rate of refrigerant	kg/h	150.94
Compressor power	kW	1.67
Vapor flow rate at compressor inlet	m3/h	26.10
Liquid flow rate at valve inlet	dm3/h	113.58

Fig. 4 : Example : cycle A. Energy analysis.

CYCLE COMPARISON

THERMOFLUID®

Cycle : A

File : MachineA

FLUID		R 12	R134a
Compressor exhaust pressure	bar abs	7.65	7.90
Condenser inlet temperature	°C	30.00	30.00
Compressor inlet pressure	bar abs	0.95	0.80
Evaporating temperature	°C	-30.00	-30.00
Compression ratio	ratio	8.05	9.87
Volumetric production at condenser	kJ/m3	888.62	791.87
Volumetric production at evaporator	kJ/m3	689.75	629.88
Volumetric work of compressor	kJ/m3	230.18	203.06
Compressor exhaust temperature	°C	54.15	48.28
Condensing power	kW	6.44	6.29
Evaporating power	kW	5.00	5.00
Mass flow rate of refrigerant	kg/h	150.94	117.27
Compressor power	kW	1.67	1.61
Vapor flow rate at compressor inlet	m3/h	26.10	28.58
Liquid flow rate at valve inlet	dm3/h	113.58	95.34

Fig. 5 : Example : cycle comparison (R12 and R134a).