MATHEMATICAL AND COMPUTER MODELS FOR THERMODYNAMIC PROPERTIES OF METHANE (R-50), ETHYLENE (R-1150) AND PROPYLENE (R-1270)

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ABSTRACT

A set of computer methods for calculating densities, vapor pressures, enthalpies, internal energies and entropies of methane (R-50), ethylene (R-1150), and propylene (R-1270) to be described. Formulation and solution of equations for these thermodynamic properties to be presented first based on what published by ASHRAE. The data obtained from these subroutines showed very small and acceptable percentage errors when compared with ASHRAE data and what available in the literature. These results ensure that these subroutines are acceptable.

KEY WORDS

Thermodynamic properties, hydrocarbon refrigerants

NOMENCLATURE

symbol	Physical quantity	Sub and superscript	Meaning
P	Pressure (MPa)		
V	Specific volume (L/mol)		
ρ	density (mol/L)	C (SUB)	Critical point value
S	Entropy (J/mol.K)	O (SUB)	Datum state
T	Temperature (K)	σ (SUB)	Saturation value
U	Internal energy (J/mol)	O (SUP)	Ideal gas property
H	Enthalpy (J/mol)	' (SUP)	Saturated liquid
C_P	Heat capacity (J/mol.K)	" (SUP)	Saturated vapor

INTRODUCTION

Because of the industrial importance of methane (R-50), ethylene (R-1150), and propylene (R-1270), especially in refrigeration field, it is necessary to produce more useful and accurate computer data-based covering the thermodynamic properties of these refrigerants.

These data need to be of high accuracy consistent with reasonable access time.

For most common refrigerants, ASHRAE has published charts and tables in SI units having the best precision available from current experimental measurements. The compilation of this material was undertaken by Ritchard B. Stewart et. al. under the supervision of ASHRAE Technical Committee (ATC). The programs to be presented here are consistent with ASHRAE data [1]. A set of computer – based methods for calculating densities, vapor pressures, enthalpies, internal energies and entropies, together with simple refrigeration cycle calculations were introduced by Chan C. and Haselden G. in a paper consisting of three parts. They presented, in the first part [2], the basic equations derivations for R-11, R-12, R-13, R-13B1-R-14, R-22, R-113, R-114, and R-502 besides to Ammonia (R-707). Latter, in the second part [3], they introduced listings for a set of computer subroutines to enable these thermodynamic properties to be calculated. Finally, in third part [4], they used these subroutines in a main program calculating the performance of a simple refrigerating cycle working with these refrigerants.

In the present work a set of computer subroutines for calculating the thermodynamic properties of these refrigerants will be presented. These subroutines constructed in such a way that can be used, alone, to find the properties in a certain state. Also, they can be equipped with a main program simulating a system working with these refrigerants. The main program can call them to calculate the properties in any place or state.

THE MAIN EQUATIONS

Ideally, all thermodynamic properties can be generated from a single equation of state covering the vapor and liquid phases in conjunction with the equation of the ideal gas heat capacity and the vapor pressure equation. The calculations of the coexistence state properties depend on the nature of the equation of state. Here, the coexistence densities were calculated by simultaneous solution of the equation of state and the vapor pressure equation. This requires an iterative procedure for the saturated liquid and saturated vapor values. The functions for entropy and enthalpy may be derived from the thermodynamic relations for properties. Since the equations of state conform to Maxwell criteria, values of entropy and enthalpy may be calculated by continuous integration along isotherms through the liquid – vapor coexistence region. This eliminates the thermodynamics inconsistencies between liquid and vapor states, which often result from the use of the independent vapor pressure function in the Clapeyron equation.

1. Equation of State

The equation of state of these refrigerants are valid for vapor and liquid states and conform closely to the Maxwell criteria of equal pressures, temperatures and Gibbs functions for the coexistence states. It is a pressure explicit equation, which is an extension of the form originally proposed by Bendict, Webb and Rubin. For methane (R-50) and ethylene (1150), this equation is:

$$
\begin{aligned}
P = \rho RT &+ \rho^2 (Y_1 T + Y_2 T^{\frac{1}{2}} + Y_3 + Y_4 / T + Y_5 / T^2 + Y_6 / T^3 + Y_7 / T4) \\
&+ \rho^3 (Y_8 T^2 + Y_9 T + Y_{10} + Y_{11} / T + Y_{12} / T^2) \\
&+ \rho^4 (Y_{13} T^2 + Y_{14} T + Y_{15} + Y_{16} / T + Y_{17} / T^2) \\
&+ \rho^5 (Y_{18} T^2 + Y_{19} T + Y_{20} + Y_{21} / T + Y_{22} / T^2) \\
&+ \rho^6 (Y_{23} / T + Y_{24} / T^2) \; + \rho^7 (Y_{25} / T + Y_{26} / T^2) \\
&+ \rho^8 (Y_{27} / T + Y_{28} / T^2) \; + \rho^9 (Y_{29} / T + Y_{30} / T^2) \\
&+ \rho^{11} (Y_{31} / T + Y_{32} / T^2) \\
&+ \rho^3 (Y_{33} / T^2 + Y_{34} / T^3 + Y_{35} / T^4) EXP(-\gamma \rho^2) \\
&+ \rho^5 (Y_{36} / T^2 + Y_{37} / T^4) EXP(-\gamma \rho^2) \\
&+ \rho^7 (Y_{38} / T^2 + Y_{39} / T^3) EXP(-\gamma \rho^2) \\
&+ \rho^9 (Y_{40} / T^2 + Y_{41} / T^3 + Y_{42} / T^4) EXP(-\gamma \rho^2) \\
&+ \rho^{11} (Y_{43} / T^2 + Y_{44} / T^3 + Y_{45} / T^4) EXP(-\gamma \rho^2) \\
&+ \rho^{13} (Y_{46} / T^2 + Y_{47} / T^3 + Y_{48} / T^4) EXP(-\gamma \rho^2) \\
&+ \rho^{15} (Y_{49} / T^3 + Y_{50} / T^4) EXP(-\gamma \rho^2) \qquad \ldots \; (1)
\end{aligned}
$$

Where, $\gamma = 1/\rho_C^2$.

For propylene (R-1270), the equation of state is:

$$
\begin{aligned}
P/\rho RT = {} & 1+\omega(y_1\tau+y_2\tau^2+y_3\tau^3)+\omega^2(y_4+y_5\tau+y_6\tau^2)+\omega^3(y_7\tau^2+y_8\tau^3) \\
& +\omega^4(y_9/\tau+y_{10}+y_{11}\tau+y_{12}\tau^3)+\omega^5 y_{13}\tau^3+\omega^6 y_{14}\tau^3+\omega^7 y_{15}\tau^3 \\
& +\omega^2\exp(-\omega^2)[y_{16}\tau^5+\omega^2 y_{17}\tau^5+\omega^4 y_{18}\tau^3+\omega^6 y_{19}\tau^3 \\
& +\omega^8 y_{20}\tau^3+\omega^{12} y_{21}\tau^4) \qquad \ldots (2)
\end{aligned}
$$

Where $\omega = \rho/\rho_C$ and $\tau = T_C/T$.

Since the equation of state is explicit in pressure, it has to be solved iteratively if the density is unknown. Thus, the density values required in enthalpy and entropy calculation can only be obtained by numerical methods.

The binary search method was considered here. It iterates in pressure and it is shown in the flowchart in figure 1. In the binary search method, the new estimate is obtained by adding a positive or negative increment depending on the approach to convergence to the old value. When the desired value is within the range of the increments, the increment is halved successively until the tolerance is met. This method was stable and proved robust under all conditions. This method was adopted therefore for all regions of refrigerant state in the present work.

2. The Vapor Pressure Equation

The vapor pressure equation for methane (R-50) and propylene (R-1270) is:

$$\ln(P_\sigma / P_C) = (T_C / T)\sum_{i=1}^{21} B_i (1 - \frac{T}{T_C})^{\frac{i}{2}} \quad \ldots (3)$$

For ethylene (R-1150), the vapor pressure equation is:

$$\ln(P_\sigma / P_0) = B_1 + B_2 X + B_3 X^2 + B_4 X^3 + B_5 X^4 + B_6 X (1 - X)^\gamma \quad (4)$$

Where: $X = [1-(T_t / T)]/[1-(T_t / T_C)]$,

$\gamma = B_7$ (for this equation), and $P_0 = 0.101325$ MPa. Where T_t is the triple point temperature.

3. The Ideal Gas Heat Capacity

The ideal gas heat capacity equation for methane (R-50) is:

$$C_P^0 / 4R = \sum_{i=1}^{6} C_i T^{i/3} + C_7 T^3 + C_8 T^4 + C_9 u^2 e^u / (e^u - 1)^2 \quad \ldots (5)$$

Where, $u = C_{10} / T$.

For ethylene, this equation is:

$$C_P^0 / R = \sum_{i=1}^{7} C_i T^{(i-4)} + C_8 u^2 e^u / (e^u - 1)^2 \quad \ldots (6)$$

Where, $u = C_9 / T$.

And for propylene, this equation is:

$$C_P^0 / R = \sum_{i=1}^{5} C_i \tau^{(1-i)} + C_6 \tau^2 + C_7 u^2 e^u / (e^u - 1)^2 \quad \ldots (7)$$

Where, $u = C_8 \tau$ and $\tau = T_C / T$.

4. Saturated Liquid Density Equation

The saturated liquid density equation for methane (R-50) is:

$$\ln(\rho' / \rho_C) = \sum_{i=1}^{4} D_i \tau^{i\gamma} + D_5 \tau^{9\gamma} + D_6 \ln(T / T_C) \quad \ldots (8)$$

Where $\gamma = D_7$ (for this equation).

For ethylene (R-1150), this equation is:

$$\rho^{'} / \rho_C = \sum_{i=1}^{24} D_i \tau^{(i-11)/3} + D_{25} \ln(T/T_C) \qquad \dots (9)$$

For propylene (R-1270), this equation is:

$$\ln(\rho^{'} / \rho_C) = \sum_{i=1}^{6} D_i \tau^{(i+2)/6} + D_7 \tau^{\frac{13}{6}} \qquad \dots (10)$$

Where $\tau = (T_C - T)/T_C$ for equations (8), (9) and (10).

5. Saturated Vapor Density Equation

The saturated vapor densities equations are:

For methane:

$$\ln(\rho^{''} / \rho_C) = \sum_{i=1}^{4} E_i \tau^{i\gamma} + E_5 \tau^{9\gamma} + E \ln(T/T_C) \qquad \dots (11)$$

For ethylene:

$$\ln(\rho^{''} / \rho_C) = \sum_{i=1}^{24} E_i \tau^{\frac{i}{3}} + E_{25} \ln(T/T_C) \qquad \dots (12)$$

For propylene:

$$\ln(\rho^{''} / \rho_C) = (T_C / T) \sum_{i=1}^{18} E_i \tau^{\frac{i}{2}} + E_{19} \ln(T/T_C) \qquad \dots (13)$$

Where $\gamma = E_7$ and $\tau = (T_C - T)/T_C$.

6. Derivation of Entropy Equation

The entropy at any state S (ρ, T) for these refrigerants, was derived by Richard et. al. [1], from the basic thermodynamic equations and Maxwell's relationships of a one component system and to be as:

$$S(\rho,T) = S^0(T) - R\ln(\rho RT / P_0) + S^1 \qquad \ldots (14)$$

Where, S^0 is the ideal gas entropy calculated from the equations of the ideal gas heat capacity as:

$$S^0(T) = S^0(T_0) + \int_{T_0}^{T} (C_P^0 / T)dT \qquad \ldots (15)$$

Where, $S^0(T_0)$ is the ideal gas entropy at the datum state at (T_0, P_0) ($P_0 = 0.101325$ MPa) and is given at the end of this paper.

Equation (15) can be integrated using some methods of integration to be:

For methane (R-50):

$$S^0(T) = S^0(T_0) + 4R[3C_1T^{\frac{1}{3}} + \frac{3}{2}C_2T^{\frac{2}{3}} + C_3T + \frac{3}{4}C_4T^{\frac{4}{3}} + \frac{3}{5}C_5T^{\frac{5}{3}} + C_6T^2/2$$

$$+ C_7T^3/3 + C_8T^4/4 + C_9[\frac{u}{e^u - 1} - \ln(1 - \frac{1}{e^u})]]_{T_0}^{T} \qquad \ldots (16)$$

For ethylene (R-1150):

$$S^0(T) = S^0(T_0) + R[\frac{-C_1}{3T^3} - \frac{C_2}{2T^2} - \frac{C_3}{T} + C_4\ln T + C_5T + \frac{C_6T^2}{2} + \frac{C_7T^3}{3}$$

$$+ C_8[\frac{u}{e^u - 1} - \ln(1 - \frac{1}{u})]]_{T_0}^{T} \qquad \ldots (17)$$

For propylene (R-1270):

$$S^0(T) = S^0(T_0) + R[C_1 \ln T + \frac{C_2}{\tau} + \frac{C_3}{2\tau^2} + \frac{C_4}{3\tau^3} + \frac{C_5}{4\tau^4} + C_6\tau^2/2$$

$$+ C_7[\frac{u}{e^u - 1} - \ln(1 - \frac{1}{e^u})]]_{T_0}^{T} \qquad \dots (18)$$

The values of u for each refrigerant in equations (16), (17) and (18) were defined in section 2.3. The value of s^1 in equation (14) is calculated for methane (R-50) and ethylene (R-1150) from:

$$S^1 = [\sum_{i=1}^{n} Y_i (XS)_i]_0^{\rho} \qquad \dots (19)$$

And for propylene (R-1270) from:

$$S^1 = -R[\sum_{i=1}^{21} Y_i (XS)_i]_0^{\omega} \qquad \dots (20)$$

The last two equations were obtained by integrating the original differential form of S^1 using some numerical techniques as described by Richard B. et. al. [1]. The final results are given directly here

7. Derivation of Internal Energy and Enthalpy Equation:

The internal energy at any state $U(\rho,T)$ is represented by:

$$U(\rho,T) = U^0(T) + U^1 \qquad \dots (21)$$

Where $U^0(T)$, is the ideal gas internal energy and is calculated as:

$$U^0(T) = U^0(T_0) + \int_{T_0}^{T} C_P^0 dT - R(T - T0) \qquad \dots (22)$$

Where, $U^0(T_0)$, is the ideal gas internal energy at the datum temperature (T_0). Equation (22) can be integrated using some methods of integration to be:

For methane (R-50):

$$U^0(T) = U^0(T_0) + 4R[\frac{3}{4}C_1T^{\frac{4}{3}} + \frac{3}{5}C_2T^{\frac{5}{3}} + C_3T^2/2 + \frac{3}{7}C_4T^{\frac{7}{3}} + \frac{3}{8}C_5T^{\frac{8}{3}}$$

$$+ C_6T^3/3 + C_7T^4/4 + C_8T^5/5 + C_9Tu/(e^u - 1)]_{T^0}^{T} - R(T - T_0) \qquad (23)$$

For ethylene:

$$U^0(T) = U^0(T_0) + R[-\frac{C_1}{2T^2} - \frac{C_2}{T} + C_3\ln T + C_4T + \frac{C_5}{2}T^2 + \frac{C_6}{3}T^3$$

$$+ \frac{C_7}{4}T^4 + \frac{C_8uT}{e^u - 1}]_{T_o}^{T} - R(T - T_0) \qquad \ldots (24)$$

For propylene:

$$U^0(T) = U^0(T_0) + R[C_1T + \frac{C_2T}{2\tau} + \frac{C_3T}{3\tau^2} + \frac{C_4T}{4\tau^3} + \frac{C_5T}{5\tau^4} - C_6T_C\tau$$

$$+ \frac{C_7uT}{e^u - 1}]_{T_o}^{T} - R(T - T_0) \qquad \ldots (25)$$

The value of U^1 in equation (21) is calculated for methane (R-50) and ethylene (R-1150) from:

$$U^1 = [T\sum_{i=1}^{50}Y_i(XU)_i - \sum_{i=1}^{50}Y_i(XS)_i]_0^{\rho} \qquad \ldots (26)$$

For propylene (R-1270):

$$U^1 = RT[\sum_{i=1}^{21}Y_i(XU)_i - \sum_{i=1}^{21}Y_i(XS)_i]_0^{\omega} \qquad \ldots (27)$$

The last two equations were obtained by integrating the original differential form of U^1 using some numerical techniques as described by Richard B. et. al. [1]. The final results are given directly here.

For ideal gas, it can be shown that:

$$H = U + P / \rho \qquad \ldots (28)$$

This equation will be adopted in the present work to calculate the enthalpy. The coefficients of equations (1) up to (28) are given in the end of this paper. The coefficients of equations (1) up to (28) are given in the end of this paper.

PROGRAM LISTINGS

In the current section, the full listings will be given in standard Fortran IV language and sufficient details will be given to enable readers with modest experience of programming to use them.

The computational scheme is built up of subroutines and the calculation of various derived properties calls on one or more of them. This approach is efficient in the use of a machine time and allows a great deal of flexibility. A considerable number of written statements are included so that the output is readily intelligible. The subroutines are listed in table 1. They are in a logical sequence in which the latter subroutine draws on the early one.

Comments on The Subroutines

Subroutine MKMID enables the constants of the equations to be read from opened files containing these constants. The identification number (MKM) should be given as an input data.

Subroutine MKMSATPR calculates the saturation pressure for a given temperature. Equations (3) and (4) were programmed here.

Subroutine MKMPREOS is a direct program of the equations of state. Equations (1) and (2) were programmed here.

The solution of the equations of state in subroutines MKMDENS giving the density is an iterative calculating program with a maximum of 50 iterations and a tolerance of 0.001 MPa. The tolerance can be altered to meet the required accuracy of the density.

The ideal gas heat capacity will be calculated by subroutine MKMCP which uses the equations (5), (6), and (7).

The saturated liquid density and saturated vapor density equations were programmed in subroutines MKMROL and MKMROV respectively.

Subroutines MKMENT, MKMINEN, and MKMENTH give direct execution of the entropy, internal energy and enthalpy respectively, which were formulated previously.

The Authors will be pleased to receive information regarding any errors which may be present in any of the listings given in this paper. They wish further to encourage readers who develop new design programs of general interest based on this refrigerant property package to offer them for publication in Tikrit Journal for Engineering Sciences.

DISCUSSION

The data obtained from the subroutines were compared with those tabulated in ASHRAE handbook (Thermodynamic properties of refrigerants) [1] as shown in figures 2 and 3 for vapor pressure and saturated vapor density for three refrigerants respectively as examples. They were very close and the error percentage was very small and accepted about (5%) for ethylene vapor pressure data as shown in figure 2.b except those for saturated vapor density of ethylene, there was a considerable error. Therefore, we have returned to other references. The equation given by Majid J. et. al. for this property was different with that given by ASHRAE handbook in spite of that they have reported the same results. Other thing, Richard B. and Richard T. are two common searchers in these two groups. So, it is evident that there is some mistake in the equation given by ASHRAE group, because it will never give the correct data. Therefore, the equation for this property given by Majid J. et. al. was adopted in the present work and gave an accepted results as shown in figure 3.b. Also we use the method of least squares and calculate the coefficient of correlation (R^2) as shown in figures that discussed above.

CONCLUSIONS AND RECOMMENDATIONS

In fact, this is an introductory step to a project of constructing a computer package for calculating the thermodynamic properties of a large number of refrigerants which help in developing any simulating program for any system using these refrigerants. It was concluded, as seen from the results, that this is a successful step. Hence, these subroutines are ready to be used in any systems simulation. Some recommendation will help in the future work:

1. More advanced computer language will make the work more flexible with additional facilities.
2. If the thermophysical properties are to be embedded in the same subroutines set, this will be very useful and make the advantage more satisfactory.

REFERENCES

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(5) Majid J., Richard T., Richard B., and Robert D., 1986. ((Thermodynamic Properties of Ethylene from Freezing Line to 450 K at pressure to 260 MPa)). J.Phys.Chem.Ref.Data, vol. 15, No. 2.

Table 1. Specification of the subroutines

Subroutine Name	Function	Subroutine Arguments	
		Input	Output
MKMID	Select the constants for the refrigerants chosen	$1 \le MKM \le 3$	-
MKMSATPR	Calculates the saturation vapor pressure for a given temperature	MKM,T	P_{sat}
MKMPREOS	Calculates the pressure from the equation of state for a given temperature and density	MKM, ρ, T	P
MKMDENS	Solving equation of state for density by binary search method	MKM,T,P	ρ
MKMCP	Calculates the specific heat for the ideal gas	MKM,T	C_P
MKMROLROV	Calculates the saturated vapor and saturated liquid densities	MKM,T	ρ_L, ρ_v
MKMENT	Calculates the entropy	MKM, ρ, T	S
MKMINEN	Calculates the internal energy	MKM, ρ, T	U
MKMENTH	Calculates the enthalpy	MKM, ρ, T ,P	H

Methane (R-50) Coefficients For the Equation of state and the Ancillary Functions (EQ. 1)

Y1 =	-0.109781817e-03	Y27 =	-0.3778708655e-06
Y2 =	0.2922180989e-01	Y28 =	0.1142430705e-02
Y3 =	-0.6601857312	Y30 =	-0.1897123346e-04
Y4 =	0.3638481430e+02	Y33 =	-0.5174519888e04
Y5 =	-0.3230345389e+04	Y34 =	-0.1463799200e+06
Y9 =	0.1149969120e-04	Y36 =	-0.6427443015e+02
Y10 =	0.3383659811e-02	Y37 =	0.9706448622e+05
Y11 =	-0.4958375718e+01	Y38 =	-0.1823686621
Y12 =	0.6701079269e+04	Y39 =	0.1737743599e+01
Y14 =	-0.4429870453e-06	Y40 =	-0.7991251291e-03
Y15 =	0.3419362760e-03	Y42 =	-0.1543689388e+01
Y16 =	0.2892714003	Y43 =	-0.1905462845e-06
Y20 =	0.1358412879e-04	Y44 =	0.5196375831e-04
Y23 =	-0.1168957228e-02	Y46 =	-0.2414009650e-08
Y24 =	-0.7405906394	Y47 =	0.6664696229e-07
Y25 =	0.4160529534e-04	Y48 =	- 0.1048901607e-05

Vapor Pressure (EQ. 3) ,ideal gas heat capacity (EQ. 5) other coefficient

B2 =	-0.6046852056e+01	C1=	0.2693860630e+01	P_C =	4.595 MPa
B3=	0.1345684762e+01	C2=	-0.2133673354e+01	$= \rho_C$	10.1095 mol/L
B5=	-0.6607506347	C3=	0.7992667721	T_C =	190.555 K
B10=	-0.1304019605e+01	C4=	-0.1604767002	R =	8.3143 J/mol-K
		C5=	0.1707967539e-01	T_O =	298.15 K
		C6=	-0.7855783683e-03	S_O (T_O) =	187.227 J/mol-K
		C7=	0.8559309457e-07	H_O (T_O) =	10017 90.68 J/mol
		C8=	-0.1457192860e-10		
		C9=	0.9189714010	Molecular wt	16.0430
		C10 =	0.2e+04		

Saturated Liquid density (EQ. 8) Saturated vapor density (EQ. 11)

D1=	0.9302871615	E1=	-0.1380664556e+01
D2=	0.7691940520	E2=	-0.5398778702
D3=	-0.6601505281	E3=	0.1093917514e+02
D4=	0.5984576027e-01	E4=	0.2625420566e+02
D5=	-0.8744067199e-01	E5=	0.1900373486e+02
D6=	-0.1060818575	E6=	0.3651595002e+02
D7=	0.270	E7=	0.290

* COEFFECIENTS NOT LISTED ARE ZERO.

ETHYLENE (R–1150) COEFFICIENTS FOR THE EQUATION OF STATE AND THE ANCILLARY FUNCTIONS*

EQUATION OF STATE (EQ. 1)

Y1 =	-0.2146684367e-02	Y27 =	-0.7534839269e-05
Y2 =	0.1791433723	Y28 =	0.1638171982e-01
Y3 =	-0.3675315604e+01	Y30 =	-0.3563090741e-03
Y4 =	0.3707178935e+03	Y33 =	-0.1833000783e+05
Y5 =	-0.3198282567e+05	Y34 =	-0.1805074210e+07
Y9 =	0.5809379775e-04	Y36 =	-0.4794587919e+03
Y10 =	-0.7895570825e-01	Y37 =	0.3531948275e+07
Y11 =	0.1448620376e+02	Y38 =	-0.2562571039e+01
Y12 =	0.2713774629e+05	Y39 =	0.1044308253e+03
Y14 =	-0.8647124319e-05	Y40 =	-0.1695303364e-01
Y15 =	0.1617727266e-01	Y42 =	-0.1710334225e+03
Y16 =	-0.2731527496e+01	Y43 =	-0.2054114462e-04
Y20 =	-0.2672283641e-03	Y44 =	0.6727558767e-02
Y23 =	-0.4752381332e-02	Y46 =	-0.1557168403e-06
Y24 =	-0.6255637346e+01	Y47 =	-0.1229814736e-04
Y25 =	0.4576234964e-03	Y48 =	0.4234325939e-04

Vapor pressure (EQ.4) Ideal gas heat capacity (EQ. 6) other coefficients

B1=	-0.9017286635e+01	C1=	0.5603615762e+06	PC =	5.0401 MPa
B2=	0.820957980e+01	C2=	-0.2141069802e+05	$= \rho_C$	7.634 mol/L
B3=	0.4315424145e+01	C3=	0.2532008897e+03	TC =	282.343 K
B4=	-0.1692585975e+01	C4=	0.3554495281E=01	R =	8.3143 J/mol-K
B5=	-0.1976495575e+00	C5=	-0.9951927478e-02	TO =	298.15 K
B6=	0.3446501098e+01	C6=	0.5108931070e-04	SO (TO) =	219.225 J/mol-K
B7=	0.15e+01	C7=	-0.1928667482E-07	HO (TO) =	29610 J/mol
		C8=	-0.2061703241E+02		
		C9=	0.300000000E+04	MOLECULARWEIGHT =	28.0543

Saturated liquid density (EQ. 9) Saturated vapor density (EQ. 12)

D2=	-0.1014799862e-07	E2=	-0.3406908747e+02
D3=	0.1552304908e-06	E3=	0.2611977687e+03
D5=	-0.7058385117e-05	E4=	-0.1148364560e+04
D8=	0.24910476683e-02	E5=	0.2908381711e+04
D10=	-0.1516683467	E6=	-0.4314780759e+04
D11=	0.1793379427e+01	E7=	0.3477526590e+04
D13=	0.1987935626e+01	E8=	-0.1189806411e+04
D18=	-0.1277044524e+01	E23=	0.2497246823e+03
D19=	0.1988609981e+01	E24=	-0.3038472515e+03
D20=	-0.6879413137		

*coefficient not listed are zero **PROPYLENE (R–1270)**

Coefficients for the equation of state and the ancillary functions

EQUATION OF STATE (EQ. 2)

Y1 =	0.1862482900	Y12 =	-0.2293103240e+01
Y2 =	-0.1292611017e+01	Y13 =	0.1251447761e+01
Y3 =	-0.5410160974e-01	Y14 =	-0.2810355287
Y4 =	0.1013803407e+01	Y15 =	0.2276598490e-01
Y5 =	-0.2121229225e+01	Y16 =	-0.2351596425
Y6 =	0.1526272166e+01	Y17 =	0.2209998579
Y7 =	-0.2552199159	Y18 =	0.3368050092
Y8 =	0.1314787725e+01	Y19 =	-0.2102485418e-01
Y9 =	-0.4565338888e-01	Y20 =	0.29849352090e-01
Y10 =	0.9265982864e-01	Y21 =	0.2851534739e-03
Y11 =	0.1020149653		

Vapor pressure (EQ.3) Ideal gas heat capacity (EQ. 7) Other coefficients

B2	-0.6553517503e+01	C1	0.6559138100	P_C	4.664 MPa
B3	0.9576459287	C2	0.1621655400e+02	ρ_C	5.3086 mol/L
B8	-0.4747026377e+01	C3	-0.4898063300e+01	T_C	365.57 K
B9	0.1931420851e+01	C4	0.8218546800	R	8.3143 J/mol-K
		C5	-0.5831480800e-01	T_O	298.15 K
		C6	0.2525251900e-01	S_O (T_O)	266.62 J/mol-K
		C7	-0.4703242000e+01	H_O (T_O)	13546. J/mol
		C8	0.1684494400e+01	Molecular weight	42.0804

Saturated liquid density (EQ. 10) Saturated vapor density (EQ. 13)

D1	-0.6744667590e+01	E1	-0.4492388452e+01
D2	0.1041706604e+03	E2	-0.2179788727e+03
D3	-0.3610992136e+03	E3	-0.2275816364e+02
D4	0.5703992324e+03	E4	0.1438327787e+03
D5	-0.4395392123e+03	E8	0.5311794215e+02
D6	0.1355081768e+03	E11	-0.1098555881e+01
D7	-0.1323118818e+01	E18	0.2601365261e+02
		E19	-0.2235815669e+03

* COEFFECIENTS NOT LISTED ARE ZERO.

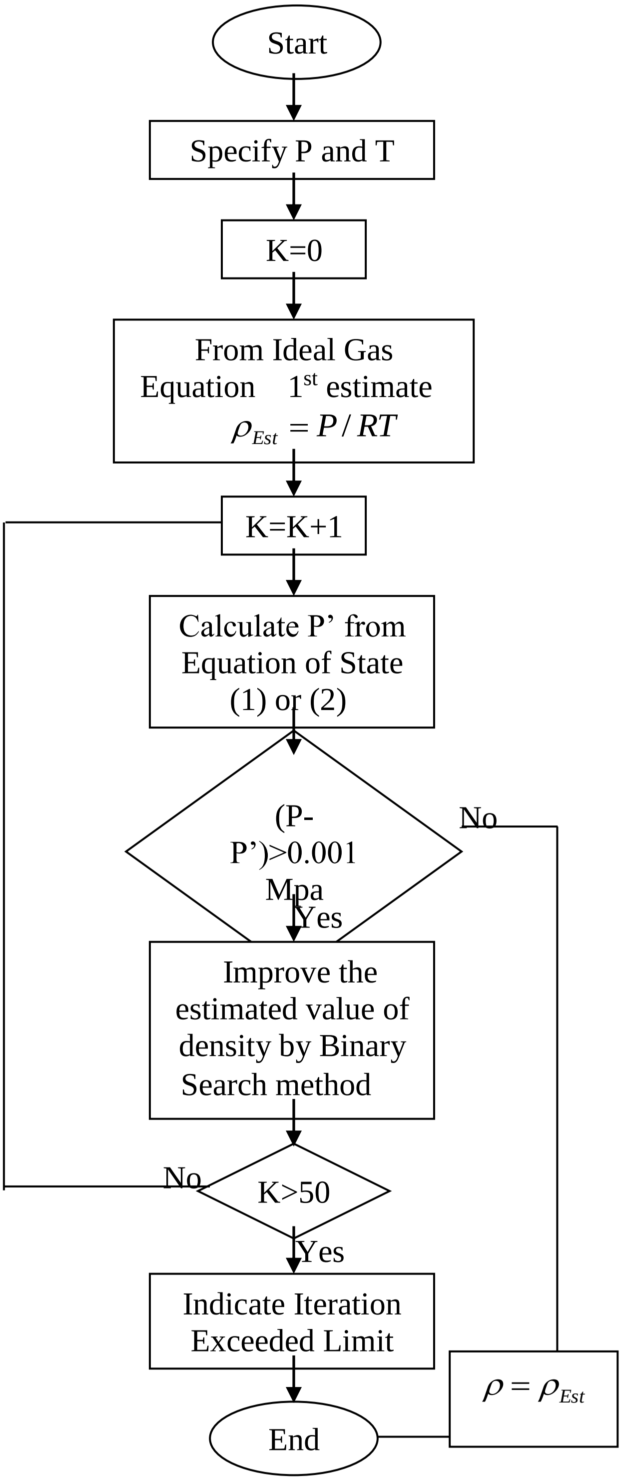
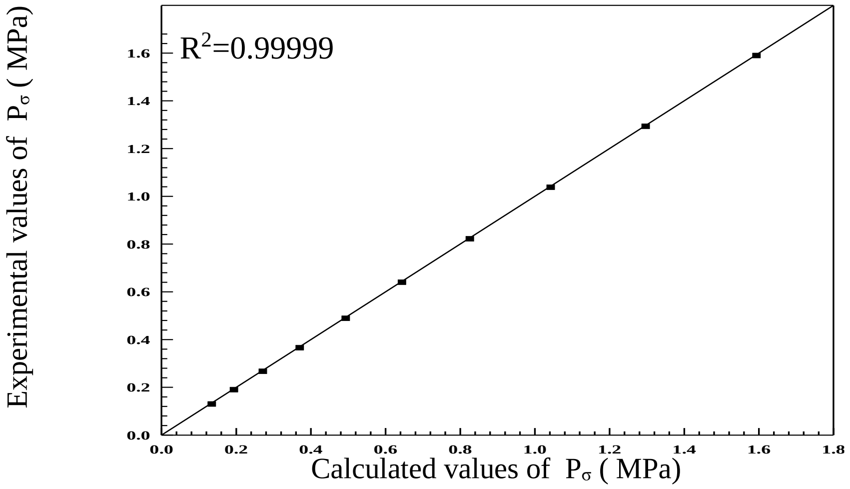
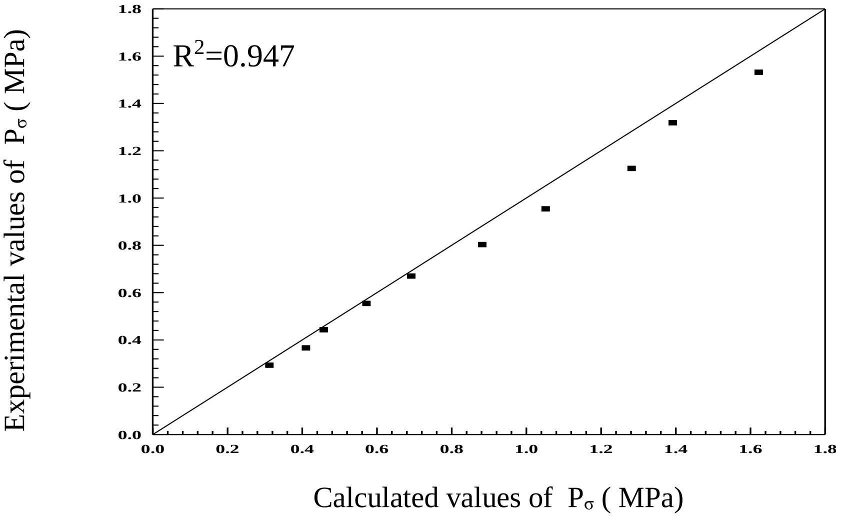


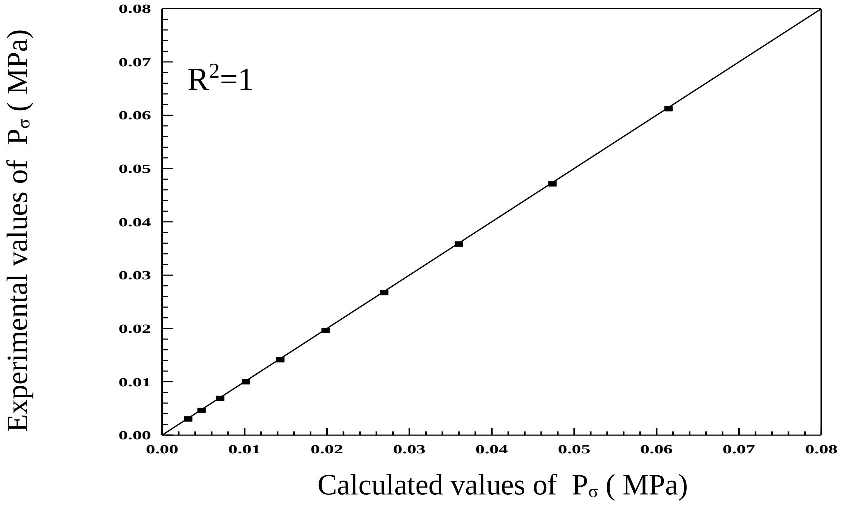
Figure (1) Flow chart of numerical solution of equation of state



c. Methane

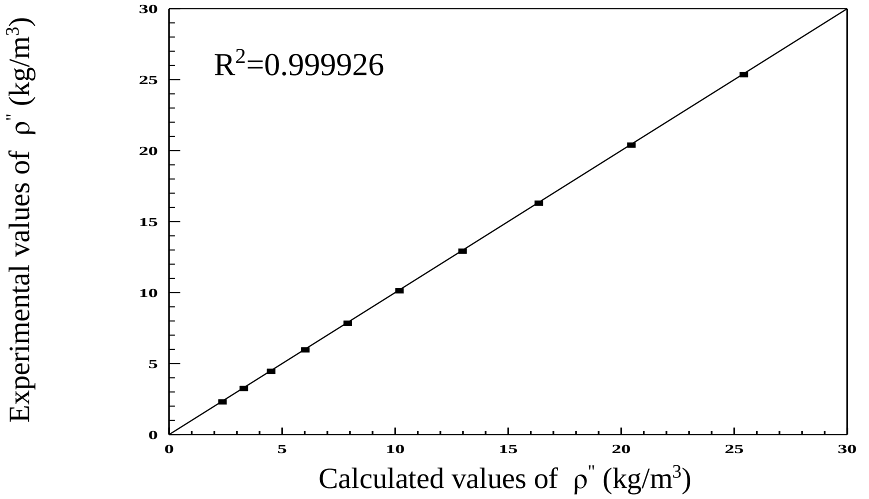


b. Ethylene

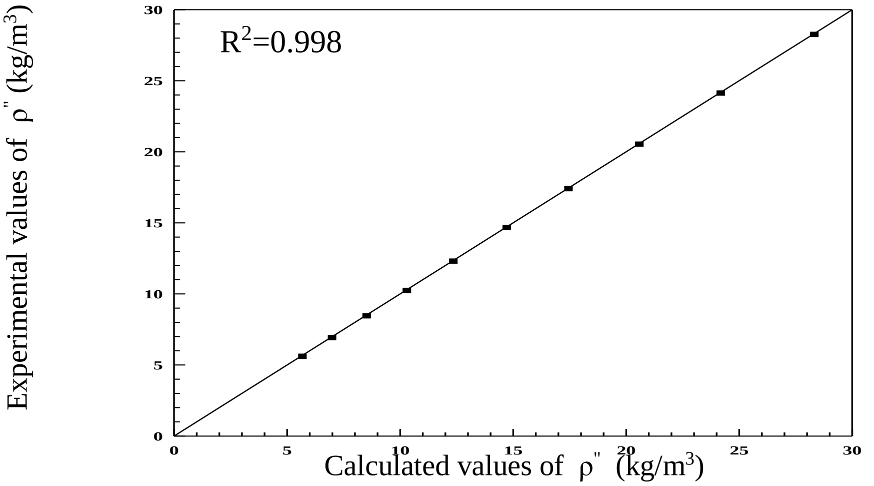


a. Propylene

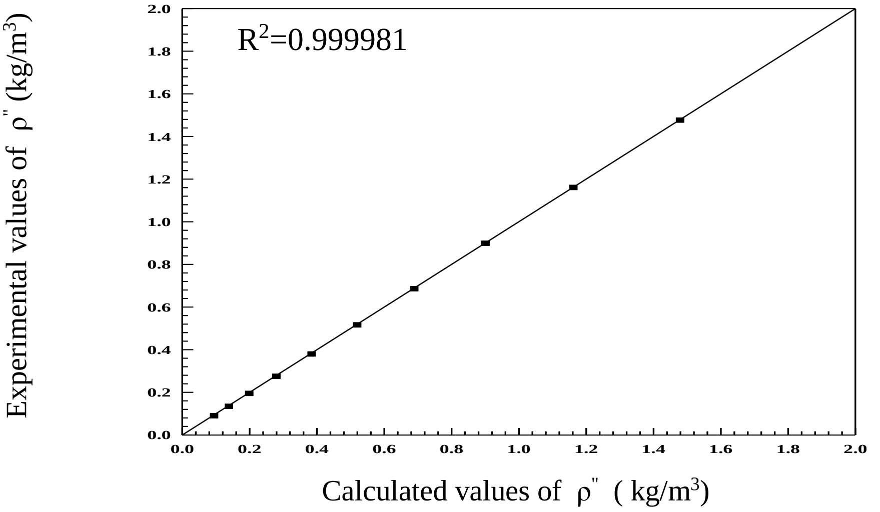
Figure (2) a compression of vapor pressure between calculated values and Experimental values.



a. Methane



b. Ethylene



c. Propylene

Figure (3) a compression of saturation vapor density between calculated values and Experimental values.

نماذج رياضية وحاسبية للخواص الثرموديناميكية للميثان والاثيلين والبروبيلين

محمد كامل محمد **نصير ضامن مخلف**

قسم الهندسة الميكانيكية – جامعة تكريت

الخلاصة

يُعنَى هذا البحث بتقديم مجموعة من البرامج الفرعية الحاسبية التي تقوم بحساب الكثافة والضغط وضغط التشبع والمحتوى الحراري والطاقة الداخلية والعشوائية (الانتروبي) لغازات الميثان والاثيلين والبروبيلين. يتم في البداية تقديم المعادلات الخاصة بتلك الخواص الثرموديناميكية مع حلها وبالاعتماد على المعادلات التي اعتمدت عليها جمعية مهندسي التدفئة والتكييف والتثليج الأمريكية (آشري). أظهرت البيانات المستخلصة من تلك البرامج الفرعية تقارباً كبيرا مع تلك المنشورة من قبل (آشري) ومع أدبيات أخرى وبنسب خطأ قليلة جدا ومقبولة. وهذا يؤكد صلاحية تلك البرامج.

الكلمات الدالة

الخواص الثرموديناميكية ، المثلجات الهيدروكاربونية