Significant Structure Theory Equation of State for the Calculation of Refrigerants Thermodynamic Properties[1]

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ABSTRACT

A new equation of state based on a modified Carnahan and Starling repulsive term designed to provide the correct close packed hexagonal volume at infinite pressure and an attractive term composed of a van der Waals potential and a Lennard-Jones potential combined using the significant structure theory of Eyring, has been developed. The NEOS was used successfully to model the thermodynamic behaviour of non-polar and polar fluids.

The new equation of state maps the critical point exactly and provides a good representation of the entire PVT map by using two adjustable parameters per pure component fitted to closely reproduce vapour pressures and liquid heat capacities. The equation has been generalized using the critical volume to map the covolume term and a simple perturbation expansion has been applied to the van der Waals potential term using Methane, n-Octane and Water as reference van der Waals potentials with acentricity and dipole moment as interpolation parameters. Results using this generalization and a modified generalization for refrigerants will be shown for the calculation of vapour pressures, saturated liquid densities, enthalpy of vapourization and isobaric heat capacities.

KEY WORDS: Equations of state; Hard Spheres; ; Lennard-Jones; Refrigerants; Significant Structure Theory

1. INTRODUCTION

At the heart of the design of any new chemical process or modification of an existing facility is the proper prediction of vapour-liquid equilibrium and thermodynamic properties like enthalpies and entropies. During the past two decades there has been an extensive attemps at adapting cubic equations of state for the modeling of virtually all mixtures encountered in the chemical industry, ranging from hydrocarbons to complex aqueous polar mixtures [1, 2, 3, 4, 5, 6, 7]. Currently, with proper care, a simple cubic equation of state can be used to predict accurate pure component vapour pressures and mixture fugacities with accuracy comparable to those predicted by a complex liquid activity coefficient model like NRTL [8] combined with empirical vapour pressure correlations.

Although proper vapour-liquid equilibrium is a fundamental step in creating a usable model for a chemical process, the need for good enthalpies, entropies and heat capacities still persist, particularly for the design of heat exchangers, compressors, expanders and turbines where the correct determination of equipment heat loads and corresponding utility fluid flows is essential. Also, the accuracy of the prediction of enthalpies and heat capacities dictate the quality of plant wide optimizations designed to diminish the consumption of energy using techniques like Pinch Analysis. Unfortunately, good vapour-liquid equilibrium prediction does not automatically translate into good thermodynamic property prediction. In a recent study, Satyro and Trebble [9] showed that advanced mixing rules derived from Gibbs and Helmholtz energy matching can produce unreliable excess enthalpies and unreasonable heat capacities at very high pressures. Knudsen and Stenby [10] evaluated the performance of several equations of state for the prediction of heat capacities and speed of sound, and they showed that a cubic equation of state can not predict heat capacities near the critical point even with parameters fitted

directly to heat capacity data. Even more surprising, they showed that at low temperatures and high densities the Lee-Kesler [11] equation of state calculates incorrect isochoric heat capacity dependency with temperature.

Since cubic equations of state are limited by their algebraic form as showed by Abbott [12] a new representation of the PVT space is required. In particular there is a need [9] for a thermodynamic model that is able to predict properties at near critical conditions, especially properties needed for the design of heat exchange equipment.

2. THEORY

The Significant Structure Theory (SST) of Eyring and co-workers [13] has been successfully used to describe thermodynamic properties of non-polar and polar substances. SST is based on a smooth interpolation using the molar volume as the parameter between a low density and a high density (solid) state. In its original formulation, considerable information per pure component was necessary, which was also dependent on the partition function being used to describe specific substances. The use of specific partition functions for different substances provided considerable accuracy and physical details about specific compounds. However, this lack of homogeneity between equations of state produced for different components made the use of SST for the prediction of mixture thermodynamic properties difficult, and the generalization of parameters very difficult at best. Nowak [14] and Hildwein and Stephan [15] showed that a precise equation of state could be created by using a single partition function based on the ideal gas state for the low density phase and a solid obeying a Kihara potential. Nowak's model was shown to produce reliable PVT mappings for a few light gases, and Stephan and Wildheim showed good results for water and ammonia. The model needed between 5 to 7 parameter per pure component, and no generalization for mixtures was published. Also, no generalization for the model parameters was suggested. Suzuki et al. [16] proposed the use of SST for modeling the

potential part of the partition function, while using a simple van der Waals model for the free volume. This produced a relatively simple equation of state, which was further enhanced to provide accurate liquid volumes. No complete generalizations for pure component parameters were proposed, and the proposed mixing rules were somewhat complex, and showed little improvement over more conventional mixing rules. Nevertheless, the model is capable of mapping the pure component critical point exactly. Suzuki's idea of using SST for the construction of the partition function potential term was used by Satyro [17], while a more rigorous expression for the free volume was sought together with a consistent boundary condition for the solid-like state at infinite pressure. In this paper only a brief description of the new equation of state (NEOS) is presented. More details are available in Satyro [17].

2.1 The New Equation of State

$$P = \frac{RT}{V}\left(\frac{V + C_1 V^0}{V - V^0}\right) - \frac{1}{V(V+d)}\left\{\begin{array}{l} a\left(1 - \frac{2V^0}{V}\right) + \\ cV^0\left[3LJ_A\left(\frac{V^0}{V}\right)^2 - 10LJ_R\left(\frac{V^0}{V}\right)^4\right] \end{array}\right\} \tag{1}$$

The repulsive term of the NEOS models the behavior of a system of hard spheres up to the hard sphere system freezing condition at a reduced density of spheres in the order of 0.66. The constant C_1 was determined to provide a good fit between the NEOS repulsive part and the results from Carnahan and Starling [18]. The final model is very simple, similar to the one proposed by Wilson [19] and provides a considerable improvement over the model proposed by Kim et al. [20] as shown in Figure 1. V^o is the sphere close packed volume, given by Eq. 2. The coefficient "a" represents the van der Waals potential energy and was made a function of temperature in the form shown in Eq. 3. The coefficient "c" represents the Lennard-Jones solid lattice potential energy, while

coefficient “b” is the covolume. Finally, coefficient “d” is an empirical modification suggested by Suzuki et al. designed to improve liquid volume predictions. LJ_A and LJ_R are the Lennard-Jones coefficients for the attractive and repulsive parts, respectively. Initial values for these coefficients were taken from Prigogine [21] and further refined to provide optimal vapour pressure predictions for Argon, and are shown in Eqs. 4 and 5.

2.2 Parameter Estimation

The parameters are determined by initially estimating a value for the parameter “b”. With “b” estimated the parameters “a_c”, “c” and “d” are estimated by using Eqs. 6, 7, 8 and 9, which represent the van der Waals conditions at the critical point. With the parameters “a_c”, “b”, “c” and “d” available, the parameters “m” and “n” are optimized to provide optimum representation of vapour pressures and isobaric heat capacities. With optimum “m” and “n” parameters the parameter “b” is optimized to provide optimum representation of saturated liquid volumes, and the process is repeated until the values of “m”, “n” and “b” do not change.

$$V^o = \frac{3b}{2\rho\sqrt{2}} \tag{2}$$

$$a(T) = a_c\left[1 + m(1-\sqrt{T_r}) + n(1-\sqrt{T_r})^2\right]^2 \tag{3}$$

$$LJ_A = \frac{7}{3} \tag{4}$$

$$LJ_R = 1.2 \tag{5}$$

$$
\begin{aligned}
\mathrm{d}_c = {} & 3P_cA'V_c^7 - 15P_cV^oA'V_c^6 + 3RT_cA'V^oV_c^5 + 27P_cA'\left(V^o\right)^2V_c^5 + \\
& C_1RT_cV^oA'V_c^5 - 10P_cR'\left(V^o\right)^2V_c^5 + 60P_cR'\left(V^o\right)^3V_c^4 - 21P_cA'\left(V^o\right)^3V_c^4 - \\
& 9RT_cA'\left(V^o\right)^2V_c^4 - 3C_1RT_c\left(V^o\right)^2V_c^4 - 18RT_cR'\left(V^o\right)^3V_c^3 + 6RT_cA'\left(V^o\right)^3V_c^3 + \\
& 6P_cA'\left(V^o\right)^4V_c^3 - 6C_1RT_cR'\left(V^o\right)^3V_c^3 - 120P_cR'\left(V^o\right)^4V_c^3 + 46RT_cR'\left(V^o\right)^4V_c^2 + \\
& 100P_cR'\left(V^o\right)^5V_c^2 + 2C_1RT_cA'\left(V^o\right)^4V_c^2 + 10C_1RT_cR'\left(V^o\right)^4V_c^2 + \\
& 6C_1RT_cR'\left(V^o\right)^5V_c - 30P_cR'\left(V^o\right)^6V_c - 30RT_cR'\left(V^o\right)^6V_c - 12C_1RT_cR'\left(V^o\right)^6
\end{aligned}
\tag{6}
$$

$$
a_c = \begin{bmatrix}
24V_cR^2T_c^2C_1\left(V^o\right)^4R' - 8V_c^6RT_cP_cA' - 18V_c^6A'P_c^2V^o + 18V_c^5A'P_c^2\left(V^o\right)^2 + \\
21V_c^5RT_cP_cV^oA' - 3V_c^5C_1RT_cV^oP_cA' + 3V_c^5R^2T_c^2A' - 15V_c^5\left(V^o\right)^2R'P_c^2 - \\
12V_c^4RT_c\left(V^o\right)^2P_cA' + 3V_c^4R^2T_c^2C_1V^oA' - 6V_c^4R^2T_c^2V^oA' + \\
12V_c^4RT_cC_1\left(V^o\right)^2P_cA' + 24V_c^4RT_cP_c\left(V^o\right)^2R' - 6V_c^4A'P_c^2\left(V^o\right)^3 + \\
45V_c^4\left(V^o\right)^3R'P_c - 8V_c^3RT_cC_1\left(V^o\right)^3P_cA' - 45V_c^3\left(V^o\right)^4R'P_c^2 - \\
8V_c^3R^2T_c^2C_1\left(V^o\right)^2A' - 10V_c^3R^2T_c^2\left(V^o\right)^2R' + V_c^3R^2T_c^2C_1^2\left(V^o\right)^2A' + \\
17V_c^3RT_cC_1\left(V^o\right)^3P_cR' - 55V_c^3RT_cP_c\left(V^o\right)^3R' + \\
15V_c^2R^2T_c^2\left(V^o\right)^3R' - 3V_c^2R^2T_c^2C_1^2\left(V^o\right)^3A' + 15V_c^2\left(V^o\right)^5R'P_c^2 + \\
30V_c^2RT_cP_c\left(V^o\right)^4R' - 42V_c^2RT_cC_1\left(V^o\right)^3R' + 24V_cRT_cC_1\left(V^o\right)^5P_cR' - \\
6V_cR^2T_c^2C_1^2\left(V^o\right)^4R' + 10R^2T_c^2C_1^2\left(V^o\right)^5R' + 6A'P_c^2V_c^7
\end{bmatrix}
\frac{V_c^2}{\mathrm{d}_c}
\tag{7}
$$

$$
c = -\begin{bmatrix}
P_c^2V_c^6 - 9P_c^2V^oV_c^5 + 3V_c^4RT_cC_1V^oP_c + 9V_c^4RT_cV^oP_c + \\
21V_c^4P_c^2\left(V^o\right)^2 - 19V_c^3P_c^2\left(V^o\right)^3 - 3V_c^3R^2T_c^2V^o - V_c^3R^2T_c^2C_1V^o - \\
22V_c^3RT_c\left(V^o\right)^2P_c - 4V_c^3RT_cC_1\left(V^o\right)^2P_c + 12V_c^2RT_c\left(V^o\right)^3P_c - \\
6V_c^2RT_cC_1\left(V^o\right)^3P_c + 6V_c^2R^2T_c^2\left(V^o\right)^2 + 6V_cR^2T_c^2\left(V^o\right)^3C_1 + \\
6V_cRT_cC_1\left(V^o\right)^4P_c + 2R^2T_c^2C_1^2\left(V^o\right)^4
\end{bmatrix}
\frac{V_c^5}{\left(V^o\right)^3\mathrm{d}_c}
\tag{8}
$$

$$d = -\begin{bmatrix} 8P_c A' V_c^7 - 36P_c V^o A' V_c^6 + 15V_c^5 RT_c V^o A' - 24V_c^5 P_c \left(V^o\right)^2 R' + \\ 60V_c^5 \left(V^o\right)^2 P_c A' - 44V_c^4 P_c \left(V^o\right)^3 A' - 24V_c^4 RT_c \left(V^o\right)^2 A' + \\ 3V_c^4 RT_c C_1 \left(V^o\right)^2 A' + 126V_c^4 P_c \left(V^o\right)^3 R' + 10V_c^4 RT_c \left(V^o\right)^2 R' + \\ 12V_c^3 P_c \left(V^o\right)^4 A' + 12V_c^3 RT_c \left(V^o\right)^3 A' - 9V_c^3 RT_c C_1 \left(V^o\right)^3 A' - \\ 234V_c^3 P_c \left(V^o\right)^4 R' - 60V_c^3 RT_c \left(V^o\right)^3 R' + 102V_c^2 RT_c \left(V^o\right)^4 R' - \\ 18V_c^2 RT_c C_1 \left(V^o\right)^4 R' + 186V_c^2 P_c \left(V^o\right)^5 R' + 6V_c^2 \left(V^o\right)^4 RT_c C_1 A' + \\ 46V_c RT_c C_1 \left(V^o\right)^5 R' - 54V_c P_c \left(V^o\right)^6 R' - 54V_c RT_c \left(V^o\right)^5 R' - \\ 30\left(V^o\right)^6 RT_c C_1 R' \end{bmatrix} \frac{V_c}{\mathrm{d}_c} \qquad (9)$$

The subscript "c" refers to the value of the parameter at the critical point. A' and R' are defined by Eqs. 10 and 11.

$$A' = 3LJ_A \qquad (10)$$

$$R' = 10LJ_R \qquad (11)$$

The temperature dependency of the "a" term and the covolume term "b" were generalized. The former ("a_c") by using a three fluid corresponding states method based on acentric factor and dipole moment. The latter ("b") was generalized using the critical volume. The model was tested by comparing predictions to a component dataset comprising more than 270 compounds representing polar and non-polar chemicals. The results of this comparison are summarized in Table 1 and the water PVT diagram calculated using the NEOS is presented in Figure 2.

3. GENERALIZATION FOR REFRIGERANTS

The van der Waals term is generalized using a simple corresponding states method shown in Eq. 12, where the subscripts "0", "1" and "2" refer to the simple non-polar reference fluid, non-polar/complex fluid, and polar fluid respectively. w and m represent the acentric factor and dipole moment, respectively.

$$\sqrt{a} = 1 + \left\{ m_o + \frac{w}{w_1}(m_1 - m_o) + \frac{m}{m_2}\left[(m_2 - m_o) - \frac{w_2}{w_1}(m_1 - m_o) \right] \right\} \left(1 - \sqrt{T_r}\right) + \left\{ n_o + \frac{w}{w_1}(n_1 - n_o) + \frac{m}{m_2}\left[(n_2 - n_o) - \frac{w_2}{w_1}(n_1 - n_o) \right] \right\} \left(1 - \sqrt{T_r}\right)^2 \quad (12)$$

For the simple fluid we chose methane (R-50), for the complex fluid we chose hexafluoroethane (R116) and the polar fluid was chosen to be methyl chloride (R-40). The "m" and "n" constants were determined for each reference fluid by simultaneous optimization of the error in the vapour pressure and isobaric heat capacity from 0.6 to 0.95 T_r . The results are summarized in Tables 2 and 3.

Note, the selected reference components provide a reasonable range in terms of acentric factors and dipole moments as shown in Table 4.

The covolume term was also correlated, Eq. 13 as a function of the critical volume using the three reference refrigerants, and was found adequate.

$$b = 0.6125 V_c \quad (13)$$

4. RESULTS

Table 5 presents a summary of the results predicted by the generalized NEOS and the Peng-Robinson EOS [22] for several refrigerants of industrial importance.

Values from the DIPPR database [23] were used in the evaluation of physical properties. The Peng-Robinson equation of state provides better estimates for saturation vapour pressure, while the generalized NEOS provides better estimates for the saturated liquid volumes, enthalpies of vapourization and isobaric heat capacities. The NEOS provides better estimates of enthalpies of vapourization and liquid volumes close to the critical point than the Peng-Robinson EOS due to an exact mapping of the critical coordinates. Isobaric heat capacities predicted by the NEOS are good up to 0.85 T_r .

5. CONCLUSION

The generalized NEOS for refrigerants provides a reliable model for the estimation of thermodynamic properties of refrigerants up to four carbon atoms. Due to the exact representation of the critical coordinates the NEOS provides accurate enthalpy of vapourizations and saturated liquid volumes close to the critical point, while providing a better estimate than Peng-Robinson EOS for the isobaric heat capacities. The Peng-Robinson EOS provides better estimates for pure component vapour pressures.

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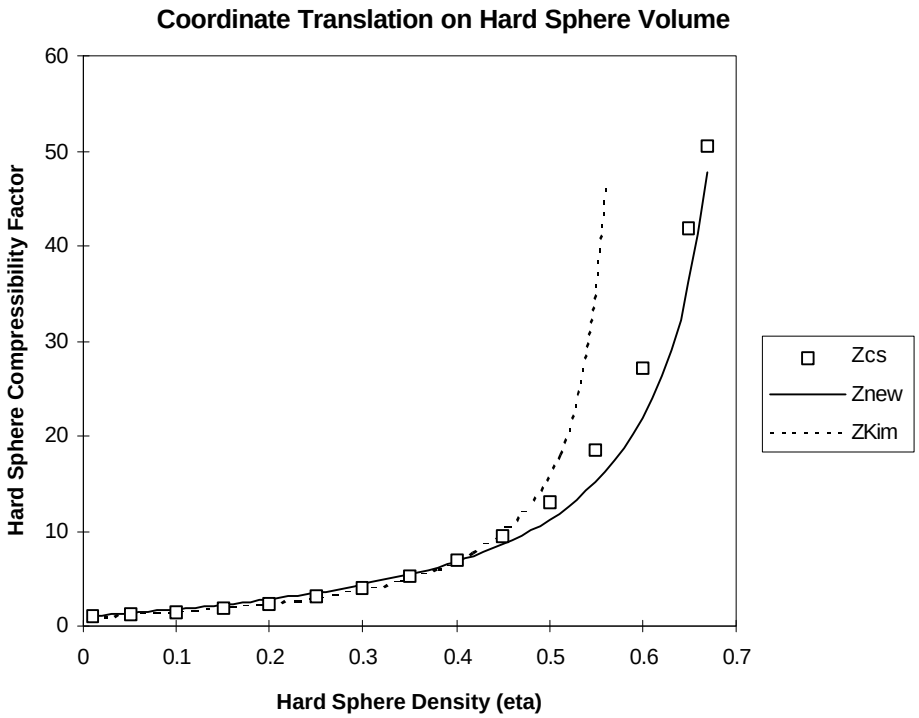

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Figure 1. Compressibility factor from Carnahan and Starling (Zcs), Kim et al. (ZKim) and NEOS (Znew).

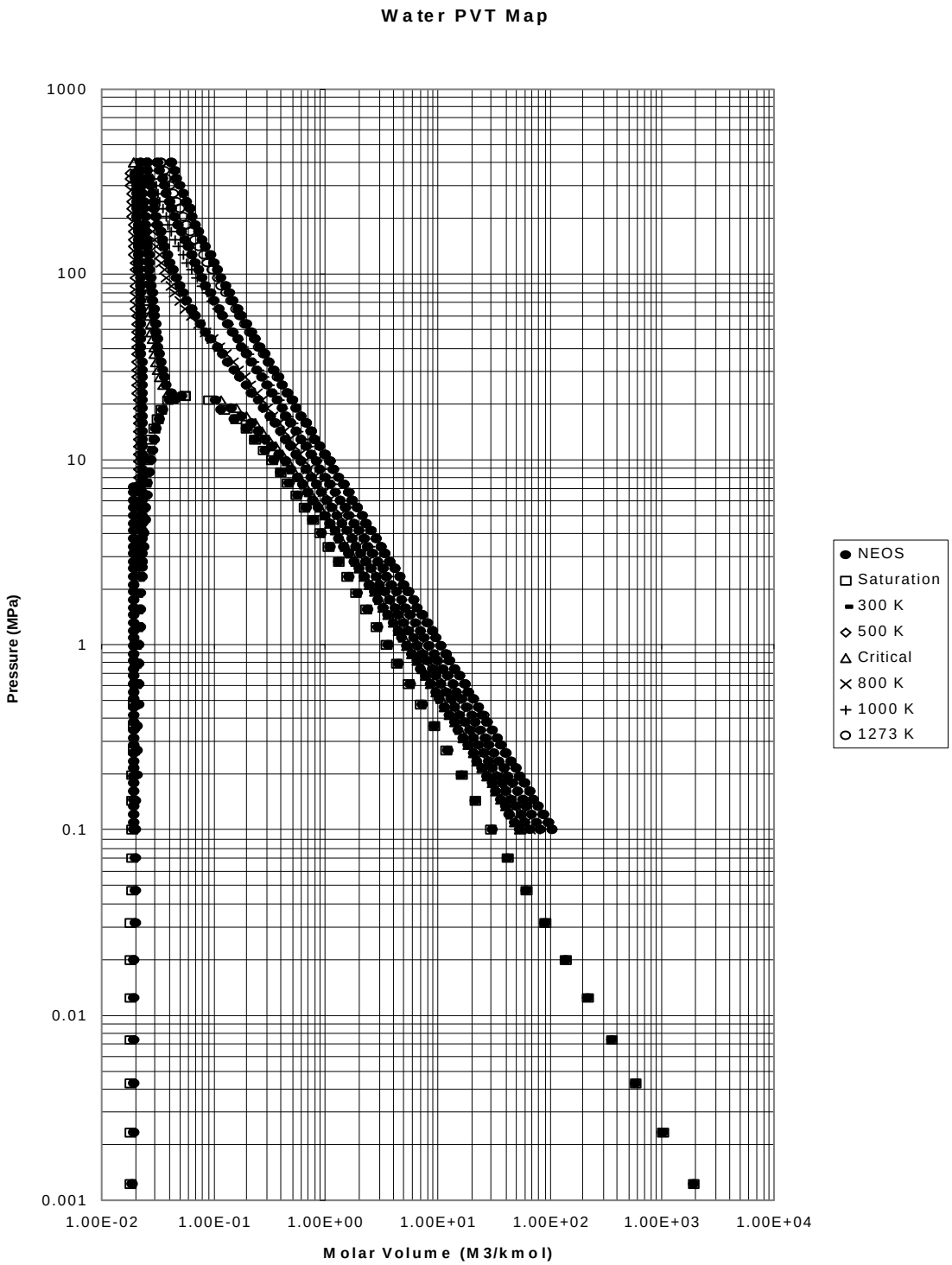

Figure 2. Water PVT diagram using NEOS.

Parameters	Vap. Pres.	Liq. Vol.	Ent. Vap.	Liq. Cp	Total
	AAD%	AAD%	AAD%	AAD%	AAD%
Optimized b, m and n	1.53	3.34	2.76	2.39	2.51
Generalized	1.52	5.19	2.48	2.47	2.92

Table 1. Summary of results for NEOS

Component	b (M^3/kmol)	m	n
Methane	6.439509E-02	-3.813470E-01	4.316067E-01
Perfluoroethane	1.381297E-01	-1.617096E-01	1.183343E+00
Methyl Chloride	8.363312E-02	-2.201348E-01	8.287850E-01

Table 2. NEOS Parameters for reference refrigerants

Component	Vap. Pres.	Liq. Vol.	Ent. Vap.	Liq. Cp
	AAD%	AAD%	AAD%	AAD%
Methane	0.64	0.75	1.61	7.90
Perfluoroethane	1.88	1.74	0.66	0.40
Methyl Chloride	0.78	1.34	1.68	10.13

Table 3. Regression Errors for Reference Refrigerants

Component	Acentric Factor	Dipole Moment (Debyes)
Methane	0.0108	0.0
Perfluoroethane	0.2451	0.0
Methyl Chloride	0.1531	1.9

Table 4. Acentric Factors and Dipole Moments for Reference Fluids

NEOS								
Component	VP	LV	DHV	CPL	VP/Tr	LV/Tr	DHV/Tr	CPL/Tr
	AAD%	AAD%	AAD%	AAD%				
Trichlorofluoromethane (R-11)	0.52	1.25	1.09	1.75	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.71
Dichlorodifluoromethane (R-12)	0.71	1.20	1.18	10.18	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.94
Chlorotrifluoromethane (R-13)	1.25	1.45	1.27	4.56	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.83
Bromotrifluoromethane (R-13B1)	0.71	1.14	1.75	3.26	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.88
Carbontetrafluoride (R-14)	1.07	3.46	1.73	1.51	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.64
Dichlorofluoromethane (R-21)	1.65	1.23	1.60	4.58	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.81
Chlorodifluoromethane (R-22)	1.77	1.66	0.85	0.98	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.63
Trifluoromethane (R-23)	2.38	3.30	3.15	18.50	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.91
1,1,2-Trichlorotrifluoroethane (R-113)	0.91	1.25	0.62	2.79	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
1,2-Dichlorotetrafluoroethane (R-114)	0.50	1.17	1.34	5.68	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.89
Chloropentafluoroethane (R-115)	0.23	2.56	1.31	0.89	0.60-0.95	0.60-0.90	0.60-095	0.60-0.88
Octafluoropropane (R-218)	1.78	1.41	2.54	5.97	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
Octafluorocyclobutane (RC-318)	2.83	2.96	1.33	1.74	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
Average	1.25	1.85	1.52	4.80				

Table 5. Results for NEOS and Peng-Robinson for various refrigerants. VP is vapour pressure, LV is saturated liquid volume, DHV is enthalpy of vapourization and CPL is isobaric heat capacity. Property/Tr show the reduced temperature range used in the error calculation.

Peng-Robinson								
Component	VP	LV	DHV	CPL	VP/Tr	LV/Tr	DHV/Tr	CPL/Tr
	AAD%	AAD%	AAD%	AAD%				
Trichlorofluoromethane (R-11)	0.29	4.61	1.52	3.05	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.71
Dichlorodifluoromethane (R-12)	0.29	4.61	1.37	10.19	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.94
Chlorotrifluoromethane (R-13)	0.42	4.99	1.56	4.56	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.83
Bromotrifluoromethane (R-13B1)	0.53	4.47	1.96	4.37	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.88
Carbontetrafluoride (R-14)	0.49	7.04	1.75	5.51	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.64
Dichlorofluoromethane (R-21)	0.29	4.61	1.37	10.19	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.81
Chlorodifluoromethane (R-22)	0.27	1.84	1.36	5.14	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.63
Trifluoromethane (R-23)	0.49	4.11	2.30	14.16	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.91
1,1,2-Trichlorotrifluoroethane (R-113)	0.92	3.80	1.34	1.54	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
1,2-Dichlorotetrafluoroethane (R-114)	0.68	4.26	1.56	7.11	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.89
Chloropentafluoroethane (R-115)	0.65	5.57	1.43	3.62	0.60-0.95	0.60-0.90	0.60-095	0.60-0.88
Octafluoropropane (R-218)	0.53	7.05	1.86	1.28	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
Octafluorocyclobutane (RC-318)	0.91	4.88	1.21	5.66	0.60-0.95	0.60-0.90	0.60-0.95	0.60-0.69
Average	0.52	4.76	1.58	5.88				

Table 5. Continued