IMPROVEMENT OF THE REDLICH-KWONG EQUATION OF STATE BY MODIFICATION OF CO-VOLUME PARAMETER

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Abstract

Cubic equations of state are widely used in phase-equilibrium calculations because of their simplicity and accuracy. Most equations of states are not accurate enough for predicting density of liquid and dense gas. A modification on the Redlich-Kwong (RK) equation of state is developed. Parameter b is modified by introducing a new parameter, β, which is a function of molecular weight and temperature. The modification gives a significant improvement over the original RK equation for predicting density. For 6538 data points of 27 compounds, the proposed equation gives only 2.8% of average absolute deviation (AAD), while the original RK and the Soave-Redlich-Kwong (SRK) equations give 11.4% and 11.7%, respectively. The proposed modification improves the performance of the RK equation for predicting vapor pressure as well. For 2829 data points of 94 compounds, the proposed modification lowers the AAD of the RK equation from 1460% down to 30.8%. It is comparable to the famous SRK equation, which give 5.8% of AAD. The advantage of the proposed equation is that it uses only critical pressure and temperature as other equations of states do, and molecular weight, which is easily calculated. Another advantage is that the proposed equation simpler than the SRK equation of state.

Keywords: *co-volume, density, equation of state, vapor pressure*

Abstrak

Persamaan keadaan bentuk kubik merupakan persamaan yang banyak digunakan dalam perhitungan keseimbangan fasa karena kemudahan dan keakuratannya. Kebanyakan persamaan keadaan bentuk kubik kurang akurat apabila digunakan untuk memprediksi density cairan dan gas bertekanan tinggi. Satu modifikasi terhadap persamaan keadaan Redlich-Kwong dikembangkan dalam penelitian ini. Parameter b dimodifikasi dengan cara memasukkan parameter baru, β, yang merupakan fungsi dari berat molekul dan temperatur. Modifikasi tersebut menghasilkan perbaikan yang sangat berarti bagi persamaan RK untuk memprediksi density. Untuk 6538 titik data dari 27 jenis senyawa, persamaan yang diusulkan dalam penelitian ini hanya memberikan kesalahan absolut rata-rata sebesar 2,8%, sementara persamaan RK asli dan persamaan Soave-Redlich-Kwong (SRK) masing-masing menghasilkan kesalahan rata-rata 11,4% dan 11,7%. Modifikasi yang diusulkan juga dapat memperbaiki kinerja persamaan RK untuk meprediksi tekanan uap. Untuk 2829 titik data dari 94 jenis senyawa, modifikasi ini dapat menurunkan kesalahan rata-rata persamaan RK dari 1460% menjadi 30,8%. Modifikasi ini hampir menyamai persamaan SRK yang sangat terkenal, yang memberikan kesalahan rata-rata sebesar 5,8%. Keunggulan dari persamaan yang diusulkan ini adalah bahawa persmaan ini memerlukan data temperature dan tekanan kritik sebagaimana persmaan keadaan kubik lainnya, dan tambahan data berupa berat molekul yang sangat mudah dihitung. Keunggulan lain adalah bahwa bentuk persamaan yang diusulkan ini lebih sederhana daripada persamaan SRK.

Kata kunci: *co-volume, densitas, persamaan keadaan, tekanan uap*

INTRODUCTION

Cubic equations of state are widely used in phase-equilibrium calculations because of their simplicity and accuracy. Every equation is claimed to be superior over the earlier ones. However, no equation fits everything. One equation is best for calculating density, but not for vapor pressure, while

another one is very accurate for predicting vapor pressure, but not for density.

Most of the equations need the critical properties data, including critical pressure and temperature, of the compounds involved in the calculations. Several equations need additional data, such as acentric factor and molar refraction. Redlich-Kwong (RK) equation of state is one of the simplest forms that needs only critical pressure and temperature:

$$P = \frac{RT}{v-b} - \frac{a}{T^{0.5}v(v+b)} \qquad (1)$$

where $\quad a = 0.42748\dfrac{R^2 T_c^{2.5}}{P_c} \qquad (2)$

$$b = 0.08664\frac{RT_c}{P_c} \qquad (3)$$

However, this equation is not accurate enough for density and phase-equilibria calculations, including vapor pressures and solubility of solids in supercritical fluids (Ratnawati *et al*, 1999; 2001; 2005; Ratnawati, 2004b).

Many modifications have been made for the RK equation of state, such as what was done by Soave (1972). Soave replaced the term $T^{0.5}$ of the RK equation of state by a function α involving temperature and acentric factor. The parameter was formulated to make the equation fit the vapor pressure data of hydrocarbons. The parameter was modified later by Graboski and Daubert (1978) with the result

$$\alpha = \left[1 + \left(0.48508 + 1.55171\omega - 0.1561\omega^2\right)\left(1 - T_r^{0.5}\right)\right]^2 \ (4)$$

The RK equation of state modified by Soave and further improved by Graboski and Daubert is known as the Soave-Redlich-Kwong (SRK) equation of state.

Another modification was proposed by Riazi and Mansoori (RM) (1993). Unlike Soave, Riazi and Mansoori focused their modification on parameter *b*. Parameter *b* of an equation of state is the repulsion parameter which is also called effective molecular volume or co-volume. Van der Waals theorized the parameter to be four times the actual volume of the molecules. This parameter plays a very important role in density calculation, especially for liquid and dense gas. Riazi and Mansoori stated that parameter *b* is more effective for calculating liquid densities because it represents the volume of molecules. For liquid and dense gas systems in which the free space between molecules decreases, the role of parameter *b* becomes more important than that of *a*. For low-pressure gases, parameter *b* is less important than *a* because the spacing between molecules increases and the attraction energy prevails.

Riazi and Mansoori (1993) modified parameter *b* using the molecular theories of perturbations and molar refraction, *Rm*. Molar refraction represents the volume occupied by molecules per unit mole. Because *Rm* and *b* have the same physical meaning, they concluded that *b* must be a function of R_m. They

modified parameter *b* by inserting a new parameter, β, which is a function of *Rm*,

$$b = 0.08664\frac{RT_c}{P_c}\beta \qquad (5)$$

where

$$\beta^{-1} = 1 + \left[0.02\left\{1 - 0.92\exp\left(-1000\left|T_r - 1\right|\right)\right\}\right.$$
$$\left. - 0.035\left(T_r - 1\right)\right]\left(\frac{Rm}{Rm_{ref}} - 1\right) \qquad (6)$$

The RM was proved to be more accurate than the original RK equation of state for predicting densities of liquids and supercritical fluids. For 6054 data points of 27 substances, this equation gives only 1.8% average absolute deviation (AAD) (Ratnawati, 2004a). However, the modification makes the equation does not satisfy the condition of criticality:

$$\left(\frac{\partial P}{\partial V}\right)_{T_c,P_c} = \left(\frac{\partial^2 P}{\partial V^2}\right)_{T_c,P_c} = 0 \qquad (7)$$

This is due to the functional form of β, which also causes the equation to have discontinuity at critical point.

The aim of this research is to develop a better modification of the RK equation of state. The modification is intended to improve the performance of the equation for predicting density of dense fluid, including liquid and dense gas, while maintaining the criticality conditions and its continuity at all conditions.

Model Development

The RM equation cut the AAD of the original RK equation of state for predicting densities of 27 compounds from 11.6% down to 1.8%. However, Riazi and Mansoori used molar refraction, which is not always available, especially for heavy-molecular weight compounds.

In this research, parameter *b* is proposed to be a function of molecular weight. It is based on the fact that molar refraction is linearly correlated to molecular weight regardless the kind of the compound is, as it is shown in Figure 1 below.

The functional form of β takes the form of that of the RM equation but in a simpler presentation:

$$\beta^{-1} = \left\{1 + \left[-2.6736 \times 10^{-2}\right.\right.$$
$$\left.\left. + 8.0454 \times 10^{-3}\left(\frac{M}{M_{ref}} - 1\right)\right]\left(1 - T_r\right)\right\}^2 \qquad (8)$$

where M_{ref} is the molecular weight of helium as the reference compound. The functional form of β is even simpler than that of parameter α of the SRK equation of state. The modified equation is then used to calculate densities as well as vapor pressures of various compounds along with the original RK and the SRK equations of state.
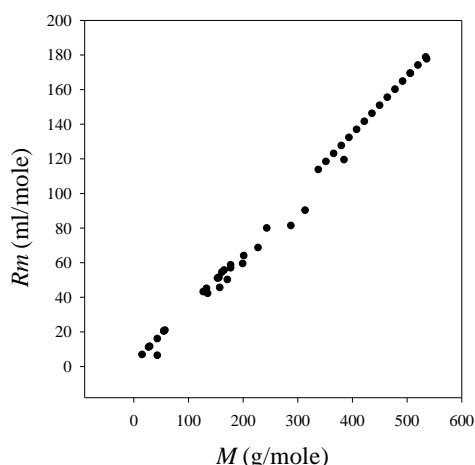
Figure 1. Relation between molecular weight and molar refraction

RESULTS AND DISCUSSIONS

The densities of various compounds were predicted using the RK, the SRK, and the proposed equations of state. The AAD of the three equations are presented in Table 1.

The results presented in Table 1 show that the proposed modification gives improves the accuracy of the original RK equation for predicting density of liquids and dense gases. For 6538 data points of 27 compounds at various conditions, this equation gives 2.8% of AAD, much lower than the original RK equation which gives 11.4% of AAD. It proves that parameter b is effective for calculating density of liquids and dense gases.

On the other hand, the SRK equation of state does not show any improvement over the original RK equation of state. For entire data, this equation gives 11.7% of AAD, a slightly higher than that of the original RK equation of state.

Table 1. The deviation of various equations of state for predicting densities of various liquids and supercritical fluids

Compound	T range (K)	P range (bar)	n	% AAD[*]			Ref.
				Prop	RK	SRK	
Helium	373-1273	5-200	55	1.9	1.3	1.0	Perry *et al*, 1997
Neon	100-1000	40-1000	72	0.8	1.6	1.2	Perry *et al*, 1997
Methane	200-500	60-500	53	1.0	1.0	2.0	Pan *et al*, 1995; Perry *et al*, 1997
Ethane	350-700	60-500	47	1.7	1.9	1.1	Perry *et al*, 1997
Propane	280-440	10-2000	206	3.5	5.3	6.1	Glos *et al*, 2004; Miyamoto *et al*, 2007
Propylene	95-340	20-120	60	2.4	6.8	7.9	Glos *et al*, 2004
n-Butane	450-750	40-2400	60	3.0	5.1	5.4	Perry *et al*, 1997
Isobutane	224-380	1-2000	179	2.9	4.8	5.4	Wacker *et al*, 1945; Miyamoto & Uematsu, 2006; Glos *et al*, 2004
1-Butene	195-283	1	8	0.8	8.3	9.8	Wacker *et al*, 1945
cis-2-Butene	242-283	1	5	3.1	10.5	11.9	Wacker *et al*, 1945
n-Pentane	180-440	1-5000	1536	1.7	9.7	10.4	Frenkel *et al*, 1997
n-Hexane	230-490	1-5000	1321	2.9	11.5	12.0	Frenkel *et al*, 1997
n-Heptane	200-573	1-5000	1473	3.0	13.4	14.0	Frenkel *et al*, 1997
n-Nonane	303-573	50-5000	324	3.4	15.8	16.2	Carmichael *et al*, 1953; Doolittle, 1964
n-Undecane	303-573	50-5000	10	4.7	19.1	19.8	Doolittle, 1964
n-Tridecane	303-573	50-5000	70	5.1	18.2	18.4	Doolittle, 1964
n-Heptadecane	303-573	50-5000	70	7.1	17.4	17.7	Doolittle, 1964
n-Eicosane	323-573	50-5000	60	6.6	26.4	26.6	Doolittle, 1964
n-Triacontane	373-573	50-5000	50	6.1	32.4	32.6	Doolittle, 1964
n-Tetracontane	373-573	50-5000	50	7.7	47.7	47.8	Doolittle, 1964
Carbon dioxide	320-700	75-1000	40	11.7	59.4	59.5	Angus *et al*, 1976
α-Pinene	293-323	1	755	2.4	3.2	2.0	Ribeiro & Gabriela, 1990
β-Pinene	293-323	1	7	8.5	17.2	18.6	Ribeiro & Gabriela, 1990
p-Cymene	293-333	1	7	6.7	18.6	20.1	Ribeiro & Gabriela, 1990
Limonene	293-323	1	7	6.6	18.5	20.0	Ribeiro & Gabriela, 1990
Lauric acid	322-383	1	7	7.1	18.7	20.2	Noureddini *et al*, 1992
Myristic acid	333-383	1	6	7.8	28.5	29.7	Noureddini *et al*, 1992
Overall			6538	2.8	11.0	11.3	

[*] $\%\,AAD = \dfrac{1}{n}\sum\limits_{i=1}^{n}\left|\dfrac{\rho_i^{calc}-\rho_i^{exp}}{\rho_i^{exp}}\right| \times 100\%$ with n = number of data points

It tells us that parameter *a* is not effective for calculating density of liquid and dense gas. Parameter *a* is called the attraction parameter. This parameter presents in the attraction part of an equation of state which represents forces of attraction between molecules. Molecular spacing in liquid and dense gas is so close that the repulsion force between molecules dominates over the attraction force. This is why parameter the modification *a* as in the SRK equation of state does not give any effect on the performance of the RK equation for predicting density of liquid and dense gas.

The proposed equation is used to predict vapor pressures of various compounds. For the sake of comparison, the RK and the SRK equations of state are used to predict the vapor pressure as well. The prediction results are compared to the experimental data taken from various sources. Some of the calculation results are presented in Figures 2 – 5. The average absolute deviations (AAD) of all equations of state for predicting vapor pressures are presented in Table 2.
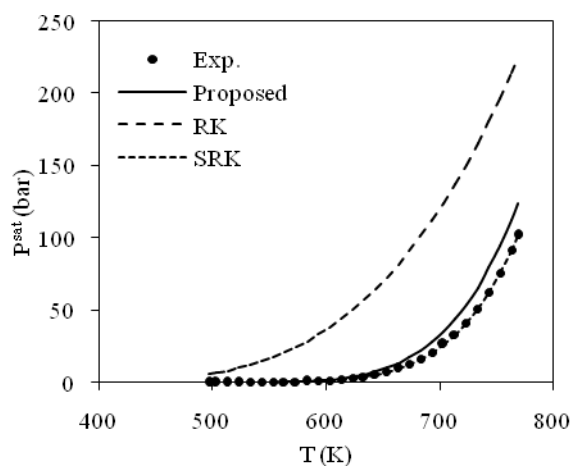

Figure 2. Vapor pressure of *n*-hexatriacontane

In Figure 2 vapor pressure of *n*-hexatriacontane is plotted against temperature. The vapor pressures predicted using the SRK equations of state, represented by dotted line, are the closest to the experimental data. It is no doubt, as the SRK equation is developed to do so. It is clear from the figure that the proposed equation, represented by solid line, is much closer to the experimental data than the RK equation. As presented in Table 2, the AADs of the RK, the proposed, and the SRK equations of state are 22.0%, 7.9% and 0.6% respectively. The results presented in Table 2 show that the improvement made by the proposed equation is more pronounced for heavier compounds. As it shown in Figure 3, the vapor pressure of *n*-hexatriacontane predicted using the proposed equation is much better than those predicted using the original RK and the MMM equations of state.
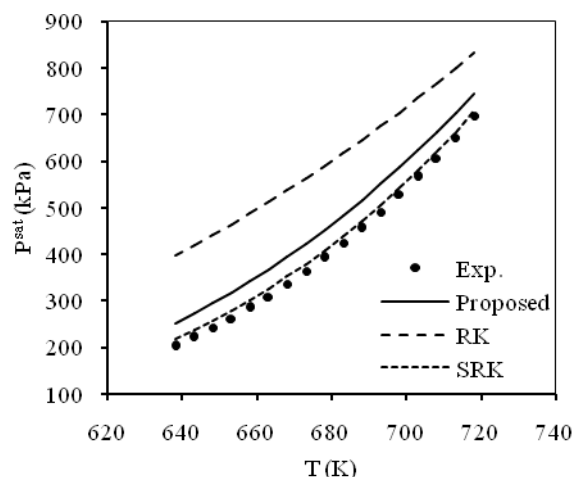

Figure 3. Vapor pressure of 1-nonadecene

Vapor pressure of one of alkenes, i.e. 1-nonadecene, is depicted in Figure 3. The proposed equation predicts vapor pressure of 1-nonadecene better than the RK equation. The proposed modification improves the AAD from 53.4% down to 15.7%.
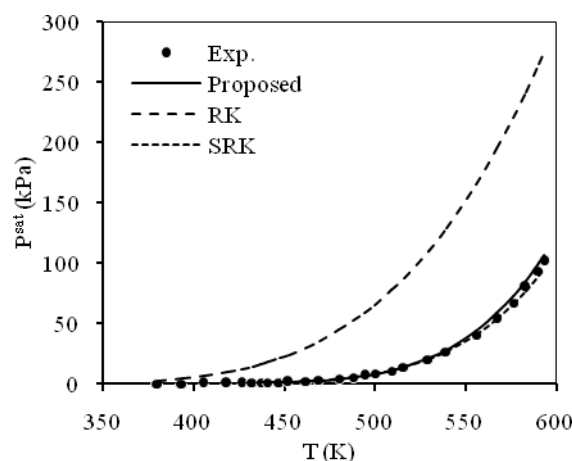

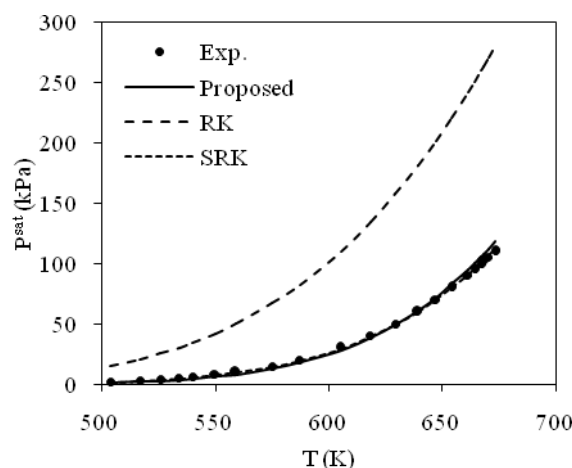Figure 4. Vapor pressure of triamylcyclohexane

Figure 5. Vapor pressure of pyrene

Figure 4 presents vapor pressure of cycloalkane, i.e. triamylcyclohexane. As it happens to alkanes and alkenes, the proposed equation is better than the RK equation. The proposed modification cuts the AAD of the original RK equation from 1837% to 16.0%. Similar phenomena also happen to aromatic compounds as it can be seen in Figure 5 which shows vapor pressure of pyrene, in which the proposed equation is very close to the experimental data and the SRK equation of state.

It is previously discussed that the proposed equation is basically formed by modifying the RK equation. It is fitted to the densities of liquids and supercritical fluids. The modification gives a remarkable improvement to the original RK equation of state for predicting density. However, the proposed modification results in a huge improvement of the RK equation of state for predicting vapor pressure. Table 2, which presents the AADs of the three equations of state for predicting vapor pressures of various compounds, shows that the modification improves the accuracy of the original RK equation of state for predicting vapor pressure. For 2829 data points of 94 compounds, the proposed equation of state gives the overall AAD of 30.8%, while the RK and the SRK equations of state give 1460.0% and 5.8%, respectively.

The calculation results found in this research indicate that parameter b is important for calculating not only density, but also vapor pressure. It is understandable, as this parameter presents in both the repulsive and the attractive parts of the equation of state. Unlike parameter b, parameter a presents only in the attractive part of the equation of state. This is why the SRK only shows improvement over the original RK equation for calculating vapor pressure, but not for density.

It should be pointed out that the proposed equation uses only uses critical pressure and temperature as other equations of states do, and molecular weight, which is easily calculated, as long as the molecular formula of the compound is known. On the other hand, the SRK equation of state uses acentric factor which is not always available, especially for heavy molecules. Another advantage of the proposed equation is that it is simpler than the SRK and RM equations of state.

Table 2. The deviation of various equations of state for predicting vapor pressures of various compounds

Compound	T range (K)	n	% AAD			Reference
			Prop.	RK	SRK	
Methane	91 -185	47	15.2	15.9	2.7	Salerno *et al*, 1986
Ethane	130 - 302	50	11.0	9.1	2.6	Salerno *et al*, 1986
Propane	150 - 360	19	7.9	22.0	0.6	Salerno *et al*, 1986
n-Butane	170 - 424	67	12.0	43.9	1.6	Salerno *et al*, 1986; Miyamoto & Uematsu, 2007; Lim *et al*, 2007
Isobutane	200 - 390	34	8.3	26.3	1.8	Salerno *et al*, 1986
n-Pentane	223 - 446	78	14.2	50.2	1.4	Salerno *et al*, 1986; Frenkel *et al*, 1997; Ewing & Ochoa, 2006
Isopentane	318 - 423	18	11.2	30.8	0.9	Frenkel *et al*, 1997
Neopentane	298 - 403	18	6.1	24.5	0.7	Frenkel *et al*, 1997
n-Hexane	227 - 483	60	19.0	96.8	2.4	Salerno *et al*, 1986
n-Heptane	271 - 523	47	26.3	114	0.8	Salerno *et al*, 1986
n-Octane	258 - 553	92	35.1	197	0.9	Salerno *et al*, 1986; Frenkel *et al*, 1997
n-Nonane	273 - 511	33	42.5	350	1.7	Salerno *et al*, 1986
n-Decane	290 - 588	54	49.4	410	1.0	Salerno *et al*, 1986; Morgan & Kobayashi, 1994
n-Undecane	348 - 500	27	50.5	295	1.7	Salerno *et al*, 1986
n-Dodecane	322 - 588	42	53.9	569	1.5	Salerno *et al*, 1986; Morgan & Kobayashi, 1994
n-Tridecane	380 - 540	27	52.7	344	1.0	Salerno *et al*, 1986; Frenkel *et al*, 1997
n-Tetradecane	373 - 588	42	47.6	394	0.7	Salerno *et al*, 1986; Morgan & Kobayashi, 1994
n-Pentadecane	409 - 577	27	49.1	379	0.8	Salerno *et al*, 1986
n-Hexadecane	378 - 594	60	52.5	652	1.1	Salerno *et al*, 1986; Morgan & Kobayashi, 1994
n-Heptadecane	433 - 610	43	50.1	488	2.5	Salerno *et al*, 1986; Frenkel *et al*, 1997
n-Octadecane	378 - 625	67	58.6	1245	2.7	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997
n-Nonadecane	423 - 639	42	55.9	789	2.5	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997
n-Eicosane	395 - 588	53	61.6	1949	10.6	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997

n-Heneicosane	393 - 630	25	61.1	4029	7.0	Frenkel *et al*, 1997
n-Docosane	411 - 653	37	64.5	3601	5.5	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997
n-Tricosane	402 - 642	24	79.9	6280	12.6	Frenkel *et al*, 1997
n-Tetracosane	418 - 688	40	66.2	4956	8.9	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997
n-Pentacosane	423 - 663	26	61.1	5992	10.9	Frenkel *et al*, 1997
n-Hexacosane	439 - 685	27	57.0	5598	11.8	Frenkel *et al*, 1997
n-Heptacosane	442 - 695	28	54.0	6818	12.7	Frenkel *et al*, 1997
n-Octacosane	448 - 703	41	53.7	6195	9.2	Morgan & Kobayashi, 1994; Frenkel *et al*, 1997
n-Nonacosane	456 - 713	27	47.4	6656	11.4	Frenkel *et al*, 1997
n-Triacontane	463 - 713	27	44.2	6407	10.9	Frenkel *et al*, 1997
n-Hentriacontane	469 - 731	28	40.0	7425	11.3	Frenkel *et al*, 1997
n-Dotriacontane	475 - 739	27	36.6	7169	10.3	Frenkel *et al*, 1997
n-Tritriacontane	481 - 747	29	33.1	8119	10.9	Frenkel *et al*, 1997
n-Tetratriacontane	487 - 754	28	29.6	7617	9.6	Frenkel *et al*, 1997
n-Pentatriacontane	492 - 762	29	26.0	8584	9.9	Frenkel *et al*, 1997
n-Hexatriacontane	497 - 769	29	23.9	7822	8.5	Frenkel *et al*, 1997
Propylene	160 - 355	38	8.4	17.5	1.4	Perry *et al*, 1997; Frenkel *et al*, 1997; Glos *et al*, 2004
1-Butene	288 - 393	19	10.6	23.3	1.0	Frenkel *et al*, 1997
1-Pentene	318 - 443	21	11.9	30.0	0.8	Frenkel *et al*, 1997
1-Hexene	358 - 483	19	14.6	36.6	1.0	Frenkel *et al*, 1997
1-Heptene	388 - 513	20	16.6	42.0	1.2	Frenkel *et al*, 1997
1-Octene	418 - 543	20	17.8	45.9	1.2	Frenkel *et al*, 1997
1-Nonene	438 - 563	19	19.5	55.0	0.7	Frenkel *et al*, 1997
1-Decene	468 - 593	20	18.0	51.2	1.2	Frenkel *et al*, 1997
1-Undecene	488 - 613	19	18.9	56.0	2.3	Frenkel *et al*, 1997
1-Dodecene	508 - 633	17	23.2	67.2	7.4	Frenkel *et al*, 1997
1-Tridecene	528 - 643	17	20.4	64.7	2.7	Frenkel *et al*, 1997
1-Tetradecene	558 - 663	17	17.1	54.2	2.5	Frenkel *et al*, 1997
1-Pentadecene	568 - 693	16	19.2	64.1	2.7	Frenkel *et al*, 1997
1-Hexadecene	352 - 693	43	38.9	948	14.8	Frenkel *et al*, 1997
1-Heptadecene	598 - 703	21	18.0	59.0	4.4	Frenkel *et al*, 1997
1-Octadecene	375 - 723	43	41.3	1164	15.6	Frenkel *et al*, 1997
1-Nonadecene	638 - 738	17	15.7	53.4	4.4	Frenkel *et al*, 1997
Cyclopropane	258 - 393	14	4.8	13.7	0.9	Frenkel *et al*, 1997
Cyclobutane	308 - 453	15	9.2	22.7	1.0	Frenkel *et al*, 1997
Cyclopentane	338 - 503	17	5.7	24.6	0.7	Frenkel *et al*, 1997
Methylcyclopentane	373 - 498	21	3.7	24.7	2.8	Frenkel *et al*, 1997
Cyclohexane	298 - 543	32	5.7	36.7	0.8	Cruiskshank & Butler, 1967; Frenkel *et al*, 1997
Methylcyclohexane	398 - 543	21	3.7	30.1	0.7	Frenkel *et al*, 1997
Cycloheptane	408 - 593	19	4.6	32.4	1.2	Frenkel *et al*, 1997
Cyclooctane	448 - 633	19	1.9	30.7	0.3	Frenkel *et al*, 1997
Dicyclohexyl	331 - 571	24	28.8	375	14.4	Myers & Fenske, 1955
Triisopropylcyclohexane	322 - 518	26	17.0	1063	5.1	Myers & Fenske, 1955
1,2-Dicyclohexyl-cyclohexane	375 - 604	26	24.5	1125	4.3	Myers & Fenske, 1955
Triamylcyclohexane	380 - 593	26	16.0	1837	3.2	Myers & Fenske, 1955
Benzene	290 - 550	25	6.3	41.7	0.8	Frenkel *et al*, 1997
Toluene	270 - 560	22	10.5	94.1	1.4	Perry *et al*, 1997; Frenkel *et al*, 1997
Ethylbenzene	433 - 598	30	21.1	47.6	10.2	Frenkel *et al*, 1997
1,2-Dimethylbenzene	453 - 613	32	10.5	36.5	1.5	Frenkel *et al*, 1997
Propylbenzene	463 - 623	28	11.6	40.5	1.1	Frenkel *et al*, 1997
1,4-Diisopropylbenzene	329 - 484	23	10.1	474	19.0	Myers & Fenske, 1955
Hexaethylbenzene	407 - 571	9	40.7	856	17.3	Myers & Fenske, 1955
Triamylbenzene	367 - 579	26	60.9	2427	17.1	Myers & Fenske, 1955
Biphenyl	343 - 740	23	16.9	338	16.4	Perry *et al*, 1997

Diamylbiphenyl	415 - 643	26	56.3	2739	11.8	Myers & Fenske, 1955
Naphthalene	353 - 523	59	26.7	182	0.6	Fowler *et al*, 1968; Frenkel *et al*, 1997
1-Methylnaphthalene	325 - 551	52	19.4	251	16.5	Frenkel *et al*, 1997
2-Methylnaphthalene	378 - 547	27	10.0	190	1.8	Frenkel *et al*, 1997
1-Ethylnaphthalene	393 - 565	27	8.3	205	4.5	Frenkel *et al*, 1997
2-Ethylnaphthalene	392 - 565	27	10.2	225	1.3	Frenkel *et al*, 1997
1,2-Dimethyl-naphthalene	402 - 542	23	8.9	270	7.2	Frenkel *et al*, 1997
Monoamylnaphthalene	350 - 562	26	24.4	1089	5.4	Myers & Fenske, 1955
Diamylnaphthalene	387 - 607	26	55.3	2249	15.9	Myers & Fenske, 1955
Dinonylnaphthalene	400 - 639	26	31.8	2222	20.2	Myers & Fenske, 1955
Anthracene	449 - 653	27	14.5	263	6.4	Frenkel *et al*, 1997
Phenanthrene	373 - 652	38	27.5	582	11.1	Frenkel *et al*, 1997
Pyrene	504 - 673	22	13.5	301	4.4	Frenkel *et al*, 1997
Tetralin	311 - 480	10	27.0	262	38.4	Perry *et al*, 1997
α-Pinene	272 - 428	10	41.6	190	37.9	Perry *et al*, 1997
β-Pinene	277 - 431	10	33.2	230	42.1	Perry *et al*, 1997
Limonene	287 - 448	10	28.7	244	25.3	Perry *et al*, 1997
		2829	30.8	1460	5.8	

CONCLUSION

New modification of parameter b of the RK equation of state is proposed. The proposed equation along with the original RK and the SRK equations of state are used to predict densities and vapor pressures of various compounds. The proposed equation is better than both the original RK and the SRK equations for predicting density. For 27 compounds with 6538 data points, the original RK, the proposed, and the SRK equations of state give overall AAD of 11.4%, 2.8%, and 11.7%, respectively. Meanwhile, the proposed equation gives a significant improvement over the original RK equation of state for predicting vapor pressure. For 2829 data points of 94 compounds, the proposed equation give 30.8%, while the RK and the SRK equations of state give 1460.0% and 5.8%, respectively. The advantage of the proposed equation is that it uses only critical pressure and temperature as other equations of states do, and molecular weight, which is easily calculated. Another advantage is that the proposed equation simpler than the SRK equation of state.

NOMENCLATURE

a equation of state parameter
b equation of state parameter
M molecular weight
M_{ref} molecular weight of reference substance (methane) = 4.0026
P pressure [kPa]
R universal gas constant
Rm molar refraction
T temperature [K]
v molar volume [l/mol]
α parameter in the SRK equation of state
β parameter in the RM and the proposed equations of state
ρ density [g/ml]
ω acentric factor

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