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Equation of state for thermodynamic properties of pure and mixtures liquid alkali metals

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ABSTRACT

We developed an equation of state based on statistical–mechanical perturbation theory for pure and mixtures alkali metals. Thermodynamic properties were calculated by the equation of state, based on the perturbed-chain statistical associating fluid theory (PC-SAFT). The model uses two parameters for a monatomic system, segment size, σ, and segment energy, ε. In this work, we calculate the saturation and compressed liquid density, heat capacity at constant pressure and constant volume, isobaric expansion coefficient, for which accurate experimental data exist in the literatures. Results on the density of binary and ternary alkali metal alloys of Cs–K, Na–K, Na–K–Cs, at temperatures from the freezing point up to several hundred degrees above the boiling point are presented. The calculated results are in good agreement with experimental data.

1. Introduction

Metals, both in liquid and in vapor states, are complicated in structure. Liquid alkali metals and their alloys are widely used in modern science and technology, for example, in nuclear energetic, and medicine [1]. These applications need the knowledge of high-temperature properties of alkali metals because these metals are heated to high-temperatures in these applications [2]. It leads to a poor accuracy in the experimental studies at high-temperatures. These considerations also make the metals suitable candidates for theoretical investigation and can be another pathway for exploring the high-temperature properties of alkali metals.

Liquids have been studied theoretically using statistical mechanics. Modern perturbation theories of liquids have been developed [3–6], based on the recognition that the structure of a dense fluid is determined primarily by the repulsive forces, so that fluids of spherical or non-spherical hard bodies can serve as useful reference systems. The influence of the attractive forces and the softness of repulsions can be treated by statistical–mechanical perturbation theory. A statistical–mechanical theory has recently been presented to derive a new analytical equation of state (EOS) of fluids [6–10].

The PC-SAFT model [10] is a theoretical-based equation of state. In contrast to many other models, PC-SAFT explicitly accounts for the non-spherical shape of a molecule, particularly of a polymer. The equation of state was already successfully applied to a huge number of systems containing gases, solvents, polymers, and co-polymers, as well as to associating systems [10].

In this study, the PC-SAFT equation of state is extended to pure and mixtures of liquid alkali metals. This equation belongs to a class of theoretically based equations of state that are formulated based on continuum space (as opposed to lattice space) liquid state perturbation theories. A comparison with other equations of state for alkali metals [11–13], the PC-SAFT equation predicted not only the liquid density of pure and mixtures, but also curves for compressed liquid density, heat capacity at constant pressure and constant volume, and isobaric expansion coefficient.

2. Theory

In the PC-SAFT equation of state, molecules are visualized to be chains of freely jointed spherical segments exhibiting attractive forces among each other, in which the pair potential for the segment of a chain is given by a square-well potential suggested by Chen and Kreglewski [14]. In this equation, non-associating molecules are characterized by three pure-component parameters: the temperature-independent segment diameter σ, the depth of the potential ε, and the number of segments per chain m.

The PC-SAFT equation is based on perturbation theories that allow dividing the interactions of molecules into a repulsive part and a contribution due to the attractive part of the potential. The repulsive interactions of this equation are described with a hard-chain expression derived by Chapman et al. [7] whereas the attractive interactions are separated into dispersive interactions

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and a contribution due to association. Here, we present only the relevant expressions of the PC-SAFT equation required in this work; the reader may consult the original papers [7,10,14] for details of the expressions concerning the PC-SAFT equation of state. For non-associating molecules, the PC-SAFT equation of state written in terms of reduced quantities of the Helmholtz energy for an N-component mixture can be expressed as

$$\tilde{a}^{\text{res}} = \tilde{a}^{\text{hc}} + \tilde{a}^{\text{disp}} \tag{1}$$

The hard-chain reference contribution is given by

$$\tilde{a}^{\text{hc}} = \bar{m}\tilde{a}^{\text{hs}} + \tilde{a}^{\text{chain}} \tag{2}$$

where $\tilde{a}^{\text{hs}}$ is the Helmholtz energy of the hard-sphere fluid, which is given on a per-segment basis by

$$\frac{a^{\text{hs}}}{RT} = \frac{1}{\xi_0}\left[\frac{3\xi_1\xi_2}{1-\xi_3} + \frac{\xi_2^3}{\xi_3(1-\xi_3)^2} + \left(\frac{\xi_2^3}{\xi_3^2} - \xi_0\right)\ln(1-\xi_3)\right] \tag{3}$$

a^{chain} is the Helmholtz energy due to the forming of chains given by

$$\frac{a^{\text{chain}}}{RT} = \sum_i X_i(1-m_i)\ln g_{ii}^{hs}(\sigma_{ii}) \tag{4}$$

and $\bar{m} = \sum_{i=1}^{N} m_i$ is the mean segment number in the mixture.

The radial distribution function of hard-sphere fluid is given by

$$g_{ij}^{\text{hs}} = \frac{1}{1-\xi_3} + \left(\frac{d_i d_j}{d_i + d_j}\right)\frac{3\xi_3}{(1-\xi_3)^2} + \left(\frac{d_i d_j}{d_i + d_j}\right)^2 \frac{2\xi_2^2}{(1-\xi_3)^3} \tag{5}$$

with

$$\xi_k = \frac{\pi}{6}\rho\sum_i X_i m_i d_i^k \quad k = 0, 1, 2, 3 \tag{6}$$

where d_i is the temperature-dependent segment diameter of component i, given by

$$d_i = \sigma_i\left[1 - 0.12\ \exp\left[\frac{-3\varepsilon_i}{kT}\right]\right] \tag{7}$$

where k is the Boltzmann constant and T is the absolute temperature. The dispersion contribution to the Helmholtz energy extended to chain molecules is given as a sum of first- and second-order contributions as

$$\tilde{a}^{\text{disp}} = \tilde{a}_1 + \tilde{a}_2 \tag{8}$$

where

$$\tilde{a}_1 = -2\pi\rho I_1(\eta, \bar{m})\overline{m^2\varepsilon\sigma^3} \tag{9}$$

and

$$\tilde{a}_2 = -\pi\rho\bar{m}C_1 I_2(\eta, \bar{m})\overline{m^2\varepsilon^2\sigma^3} \tag{10}$$

which depend on the integrals of power series of sixth-order in density,

$$I_1 = \sum_{i=0}^{6} a_i\eta^i \tag{11}$$

and

$$I_2 = \sum_{i=0}^{6} b_i\eta^i \tag{12}$$

with

$$a_i = a_{0i} + \frac{m-1}{m}a_{1i} + \frac{m-1}{m}\frac{m-2}{m}a_{2i} \tag{13}$$

$$b_i = b_{0i} + \frac{m-1}{m}b_{1i} + \frac{m-1}{m}\frac{m-2}{m}b_{2i} \tag{14}$$

Table 1
Parameters used for alkali metals.

Metal	σ (Å)	ε/k (K)	$\gamma \times 10^4$ (J/mol K^2)
Li	2.8880	2941.041	17.6
Na	3.5078	1940.862	14.6
K	4.3275	1615.121	19.7
Rb	4.6289	1494.280	24.3
Cs	5.0038	1433.099	32.2

with the universal constants a_{0i}, a_{1i}, a_{2i}, b_{0i}, b_{1i}, b_{2i} [10].

The term C_1 given in Eq. (10) can be expressed as

$$C_1 = \left(1 + Z^{\text{hc}} + \rho\frac{\partial Z^{\text{hc}}}{\partial\rho}\right)^{-1}$$

$$= \left(1 + m\frac{8\eta - 2\eta^2}{(1-\eta)^4} + (1-m)\frac{20\eta - 27\eta^2 + 12\eta^3 - 2\eta^4}{((1-\eta)(2-\eta))^2}\right)^{-1} \tag{15}$$

where Z^{hc} is the compressibility factor of the hard-chain reference contribution and $\eta = \zeta_3$ is the packing fraction. The van der Waals one-fluid mixing rules are represented by

$$\overline{m^2\varepsilon\sigma^3} = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j m_i m_j\left(\frac{\varepsilon_{ij}}{kT}\right)\sigma_{ij}^3 \tag{16}$$

and

$$\overline{m^2\varepsilon^2\sigma^3} = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j m_i m_j\left(\frac{\varepsilon_{ij}}{kT}\right)^2\sigma_{ij}^3 \tag{17}$$

which contain the conventional combining rules to determine the cross terms between a pair of different segments,

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \tag{18}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i\varepsilon_j}(1 - k_{ij}) \tag{19}$$

where k_{ij} is an adjustable interaction parameter, which is introduced to correct the segment–segment interactions of unlike chains. The three pure-component parameters of the PC-SAFT model, segment number m, segment diameter σ, and segment energy parameter ε, can be regressed by fitting pure-component data.

3. Results and discussion

The PC-SAFT equation of state is applied to Alkali metals in a wide range of pressure and temperature. All metallic systems are considered as monatomic systems ($m = 1$). Therefore, knowing two adjustable parameters σ and ε is sufficient to predict the equation of state for liquid metals. The parameters were identified for five alkali metals by correlating saturated liquid density. Table 1 shows regressed values (ε, σ) of PC-SAFT parameters. With knowing the values of ε and σ, can predict the *PVT* properties of liquid metals. Experimental data are taken from [15]. We have computed some selected thermodynamic properties of five alkali metals in liquid phase. The thermodynamic properties in question are the saturation and compressed liquid density for pure and mixtures, heat capacity at constant pressure and constant volume, and Isobaric expansion coefficient. In what follows, we will discuss in detail the results obtained for each property. We first examine the volumetric properties and then other thermodynamic properties of fluids will be discussed.

Table 2
Result for saturated liquid density of alkali metals with PC-SAFT equation of state.

Metal	ΔT (K)	[a]NP	[b]AAD (%)	AAD (%) Previous work [11]
Li	700–1700	11	2.58	0.64
Na	400–1200	9	2.03	2.07
K	400–1100	8	1.45	1.77
Rb	400–1200	9	1.59	2.67
Cs	400–1200	9	1.83	2.12
Average			1.89	1.85

[a] NP represents the number of data point's examined.

[b] AAD (%): absolute average deviation $= 100/NP\sum_{i=1}^{NP}|\rho_{i,\text{Cal.}} - \rho_{i,\text{Exp.}}|/\rho_{i,\text{Exp.}}$.

Table 3
The calculated absolute deviation for saturated liquid density of Rb compared with experimental data [15].

T (K)	p (10^{-6} MPa)	p (mol m^{-3})		Deviation (%)
		Calculation	Experimental	
400	0.1614	16,436	16,959	3.09
500	16.85	16,046	16,457	2.50
600	359.7	15,640	15,916	1.73
700	3131	15,230	15,376	0.95
800	15,660	14,818	14,854	0.25
900	54,310	14,403	14,345	0.40
1000	146,300	13,981	13,836	1.05
1100	328,400	13,547	13,312	1.76
1200	643,500	13,093	12,762	2.59
AAD (%)				1.59

4. Thermodynamic properties from equation of state

4.1. The saturation liquid density

The calculation of the density or the molar volume from the given pressure and temperature is one of the most frequently performed operations in phase equilibrium calculations. Using *P–T* data [15], we have calculated the saturation liquid density of Li, Na, K, Rb, and Cs. The results are shown in Table 2. The result for Rb as a typical example is also shown in Table 3, on which any deviation pattern is more obvious. In order to show how the equation of state passes through the experimental points, we have plotted deviation plots and the saturated liquid density in Fig. 1. Comparison of the results with previous work [11] has been shown in Table 2.

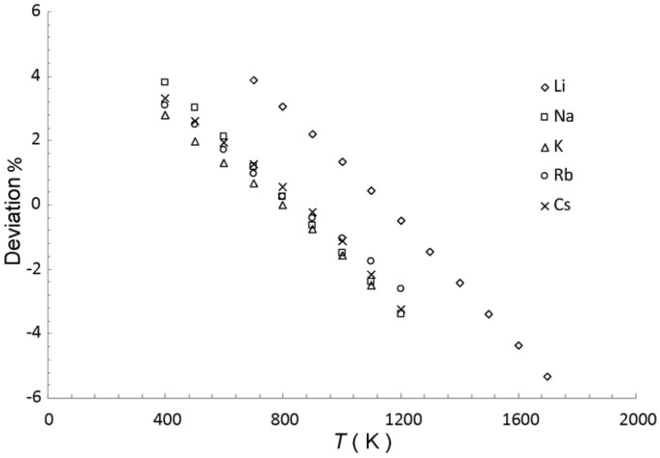

Fig. 1. Deviation plot for the predicted saturation liquid density of alkali metals compared with experiment.

Table 4
The calculated absolute deviation for the compressed liquid density of Cs compared with experimental data [15].

T (K)	p (MPa)	ρ^{exp} (mol m^{-3})	ρ^{cal} (mol m^{-3})	Deviation (%)
600	10	12,675	12,332	2.71
600	20	12,788	12,364	3.32
600	40	12,998	12,427	4.39
600	60	13,189	12,488	5.32
600	80	13,366	12,546	6.13
600	100	13,529	12,603	6.85
1000	10	10,990	10,976	0.13
1000	20	11,161	11,028	1.20
1000	40	11,469	11,126	2.99
1000	60	11,739	11,218	4.44
1000	80	11,981	11,304	5.65
1000	100	12,200.3	11,385.7	6.68
1600	10	8015	8115	1.25
1600	20	8411	8408	0.04
1600	40	9014.9	8814.2	2.23
1600	60	9484	9107	3.97
1600	80	9874	9341	5.40
1600	100	10,211	9538	6.59
AAD (%)				3.84

Table 5
Predicted results for the compressed densities of alkali metals.

Metal	ΔT (K)	Δp (MPa)	AAD (%)	AAD (%) Previous work [11]
Li	600–1600	10–100	3.30	2.62
Na	600–1600	10–100	3.15	2.00
K	600–1600	10–100	2.45	2.37
Rb	600–1600	10–100	2.93	3.83
Cs	600–1600	10–100	3.84	3.46
Average			3.13	2.87

4.2. The compressed liquid density

The ability of the present equation of state to predict *PVT* data is presented. The outcome of the density calculations of all alkali metals is gathered in Tables 4 and 5. Experimental data are taken from [16–20]. Table 5 shows comparison of the results with previous work [11]. The calculations cover the pressure range 10 MPa < p < 100 MPa and temperature range 600 K < T < 1600 K. Comparison of the results in Fig. 2, show the present equation of state is accurate for representation the compressed liquid density data for them.

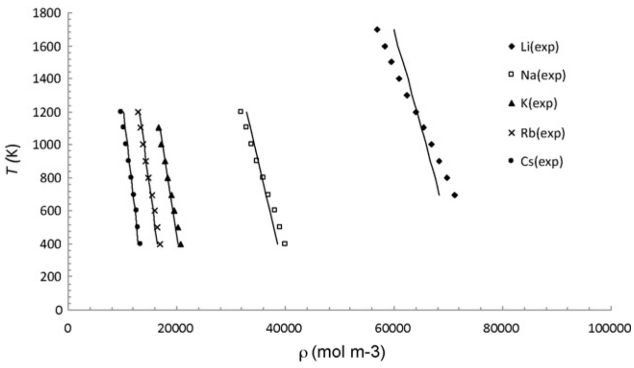

Fig. 2. Comparison between calculated and experimental results for saturated liquid density of alkali metals. The line markers show the results of the PC-SAFT equation of state and the corresponding filled ones are experimental data [15].

Table 6
Predicted results for the liquid densities of alkali metals alloy.

Alloy	ΔT (K)	Δp (MPa)	AAD (%)
0.9 K + 0.1 Cs	350–1150	1.499×10^{-10}–2.974×10^{-1}	1.60(3.22)[a]
0.8759 K + 0.1241 Cs	400–1000	6.356×10^{-10}–8.514×10^{-1}	4.51(5.58)
0.7015 K + 0.2985 Cs	400–1000	1.271×10^{-7}–1.019×10^{-1}	2.13(3.62)
0.3032 K + 0.6978 Cs	400–1000	2.725×10^{-7}–1.403×10^{-1}	2.26(4.31)
0.3 K + 0.7 Cs	350–1050	2.274×10^{-7}–2.134×10^{-1}	1.86(4.09)
0.2 K + 0.8 Cs	350–1000	2.403×10^{-10}–1.501×10^{-1}	1.95(4.12)
0.1 K + 0.9 Cs	350–1000	2.532×10^{-10}–1.597×10^{-1}	1.85(4.00)
0.1 K + 0.9 Na	600–1200	1.854×10^{-5}–2.238×10^{-1}	1.84(2.98)
0.2 K + 0.8 Na	600–1200	2.620×10^{-5}–2.252×10^{-1}	1.80(2.69)
0.319 K + 0.681 Na	600–1200	3.739×10^{-5}–2.450×10^{-1}	1.76(3.10)
0.4 K + 0.6 Na	600–1200	4.634×10^{-5}–2.654×10^{-1}	1.79(2.87)
0.5 K + 0.5 Na	600–1200	5.897×10^{-5}–2.953×10^{-1}	1.77(2.85)
0.598 K + 0.402 Na	600–1200	7.358×10^{-5}–3.277×10^{-1}	1.75(2.82)
0.7 K + 0.3 Na	600–1200	9.077×10^{-5}–3.605×10^{-1}	1.70(2.51)
0.8 K + 0.2 Na	600–1200	1.110×10^{-4}–3.925×10^{-1}	1.68(2.74)
0.9 K + 0.1 Na	600–1200	1.314×10^{-4}–4.093×10^{-1}	1.73(3.29)
0.1 Na + 0.4749 K + 0.4246 Cs	450–1000	2.036×10^{-6}–1.087×10^{-1}	5.87(7.39)

[a] Maximum deviations in parentheses.

4.3. Density of binary and ternary

We have calculated the densities of alkali metal alloys of Cs–K, Na–K, Na–K–Cs, at temperatures from the freezing point up to several hundred degrees above the boiling point. The experimental densities are taken from Ref. [21].

In this work we have generalized the correlation to the mixtures, using simplest combining rules for predicting unlike-molecule interactions from the like molecule interactions, are a geometric mean for ε and an arithmetic mean for σ. Thus, our combining rules would be:

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \tag{20}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \tag{21}$$

Analysis of the results in Table 6, shows we can acquire very good results (AAD (%) = 2.23), as same as other works [12,13] (AAD (%) = 3.02). This fact reveals that alkali metal alloys obey nearly the same two-parameter intermolecular pair potential energy functions of singlet and triplet.

4.4. Heat capacities

The estimation of caloric data such as heat capacities is important in technological application. The heat capacity at constant volume and constant pressure are determined by the derivative of Helmholtz energy and the pressure which are direct calculation from the PC-SAFT equation of state:

$$C_V(T,\rho) = -T\left(\frac{\partial^2 a}{\partial T^2}\right) \tag{22}$$

$$C_p(T,\rho) = C_V(T,\rho) + \left[\left(\frac{\partial p}{\partial T}\right)_\rho^2 \left(\frac{\partial \rho}{\partial p}\right)_T \left(\frac{T}{\rho^2}\right)\right] \tag{23}$$

The heat capacity of a liquid metal is made up of several contributions, a kinetic term, an electronic term, and a configurational term due to inter atomic forces. The kinetic term for mono atomic fluids is $3R/2$, where R gas constant. In this work PC-SAFT is use to determined the configurational term from Eq. (22). According to the Fermi–Sommerfeld theory, the contribution C^{el} from conduction electrons is given by

$$C^{\text{el}} = \gamma T \tag{24}$$

where γ is a constant for temperatures much smaller than the effective Fermi temperature [22]. For the metals being considered here the Fermi temperature is of order of 10^4 K. Therefore Eq. (24) should give a good approximation of the electronic heat capacity of these simple metals in liquid state. Values are given in Table 1.

The AAD (%) of heat capacities at constant pressure and constant volume have also been included in Table 7. The deviations are of the order of 18%, and 13%, respectively, for C_p and C_V. The maximum and minimum difference between experimental and calculated values of C_p for Rb are 11.39 J/mol K (2.72 cal/mol K) and 0.14 J/mol K (0.03 cal/mol K), and the maximum and minimum difference between experimental and calculated values of C_V for Rb are 5.86 J/mol K (1.40 cal/mol K) and 0.06 J/mol K (0.01 cal/mol K). The calculated results are in good agreement with experimental data. It is well known that for the alkali metals electronic contribution to the heat capacities is significantly large varying from 0.5 to 3.5 J/mol K. Should the electronic contributions were added to the calculated results, the agreement would have been better.

4.5. Isobaric expansion coefficient

The constant pressure coefficient of thermal expansion α of a substance is defined by the equation

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \tag{25}$$

Note that α is the fractional change in volume ($\Delta V/V$) divided by the corresponding change in temperature ΔT, and thus α has the units of per kelvin, K^{-1}. The evaluated results for thermal expansion are presented in Table 7. From table it is seen that the agreement between the theoretical and corresponding experimental values is reasonably good. The maximum differences between the calculated and experimental are $0.000077\ \text{K}^{-1}$ for Rb.

Table 7
The absolute average deviation percent of thermodynamic properties from literature values [15].

Metal	ΔT (K)	Δp (MPa)	C_V	C_P	α
Li	500–1200	0–3	–	9.13	46.00
Na	400–1200	0–8	13.06	19.57	31.94
K	400–1100	0–60	13.60	21.00	19.66
Rb	400–1000	0–60	13.45	19.50	18.95
Cs	400–900	0–60	13.20	21.77	16.57

5. Concluding remarks

There exist some similarities between fluid metals and ordinary fluids that lead us to check the present equation of state for them. For example, liquid metals can be treated as simple monatomic systems and like normal fluids. The PC-SAFT equation of state was proposed and applied to estimate the physical properties of metals up to the several hundred degrees above the boiling point for alkali metals. Model parameters σ and ε were obtained by regressing saturated liquid density data.

The thermodynamic functions of five alkali metals were calculated using a statistical–mechanical-based equation of state known as PC-SAFT on a wide *PVT* range. Perturbation theory with hard-sphere reference system is a good first approximation for the study of static properties of liquid alkali metals. The interesting point of this work is that this EOS is also suitable to employ to predict other thermodynamic properties as well as density within acceptable accuracies.

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