



Estimation and modelling of the thermodynamic properties of small alkanes at low pressure

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Abstract. In this research, some thermodynamic properties of small alkanes are estimated and modelled to evaluate the performance of the correlation equation of their second virial coefficient at low density and pressure. The studied fluids are CH₄ to *n*-C₅H₁₂. The correlation equation used is the one suggested by Zarkova *et al.* Thermodynamic properties measured are: Joule–Thomson coefficient, enthalpy, fugacity coefficient, thermal expansion and bulk modulus. In addition, Boyle temperature and Boyle volume are also estimated using the correlation. By using virial coefficients and virial equation of state, which is based on theoretical studies and statistical mechanics, a bridge is created between the microscopic and macroscopic properties that can show the non-ideal behaviour of real fluids. The obtained results show that the thermodynamic properties of the studied molecules and their deviation from the ideal state have been predicted and modelled very well by the correlation equation presented in a wide range of temperatures.

Keywords. Thermodynamic properties; alkanes; virial coefficients; correlation equation.

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1. Introduction

Alkanes represent one of the simplest important sequences of chemistry. These organic materials are considered saturated hydrocarbons and have the lowest reactivity among hydrocarbons and are of great economic importance. In addition, they are major components of fuels and petroleum lubricants and are widely used in chemistry. Pure alkanes such as hexane can be used as solvents. Alkanes are either non-polar or have very poor polarity. They are not electrically conductive and also do not polarise in an electric field. For this reason, they do not form hydrogen bonds and are not soluble in polar solvents such as water. Of course, the solubility of these materials is high in non-polar solvents. Different alkanes are miscible with each other in any proportion. Free radicals play an important role in most alkane reactions such as cracking and reforming. In this type of reaction, long chains of alkanes are converted to shorter chains and straight-chain alkanes are converted to branched ones.

Due to their importance and their wide application in chemistry, especially as raw materials for the synthesis of many organic compounds, much research has

been done to describe their thermophysical properties in a wide range of densities, pressures and temperatures experimentally and theoretically. Theoretical research has the benefit of leading to the modelling of the thermodynamic behaviour of materials. Modelling the thermophysical properties of materials is very important to predict their thermodynamic behaviour in different conditions. Using this approach, these properties can be estimated and therefore, many experiments can be avoided. In this regard, different methods of simulation, statistical approaches, *ab-initio* calculations and equations of state can be considered and used. Each of these methods has advantages and limitations. Some of them are microscopic methods and some are macroscopic ones.

For example, Haghghi *et al* used five equations of state (EOS) for predicting Joule–Thomson inversion curve for methane, ethane and propane [1]. Quinones-Cisneros *et al* modelled the density and viscosity of pure *n*-alkanes using friction theory and non-cubic equation of state [2]. Hinojosa-Gomes *et al* presented two modifications to the Peng–Robinson-fitted equation of state for pure substances like *n*-alkanes to predict their vapour pressure and density [3]. Ting

et al modelled phase equilibrium of mixtures of long-chain and short-chain alkanes using Peng–Robinson and SAFT EOSs [4]. Alfradique and Castier calculated critical points of hydrocarbon mixtures with the Peng–Robinson, SAFT and PC-SAFT EOSs [5]. Eslami suggested that the *PVT* properties of pure fluids like *n*-alkanes can be determined with reasonable accuracy from just the two scaling constants, T_{bp} and ρ_{bp} using Weeks–Chandler–Anderson EOS which is based on statistical–mechanical perturbation theory [6]. Bucker and Wagner presented a reference EOS for the thermodynamic properties of ethane [7]. Maghari and Najafi suggested a new method, namely the ‘common intersection method’ for predicting the liquid–vapour interfacial surface thickness of *n*-alkanes [8].

In this paper, thermodynamic properties of small alkanes (CH_4 to $n\text{-C}_5\text{H}_{12}$) are estimated and modelled by virial equation of state (VEOS). VEOS which is based on theoretical studies and statistical mechanics, has been used extensively to study the thermodynamic properties of gases and this approach in which the connection bridge is created between microscopic and macroscopic properties can show the non-ideal behaviour of real fluids.

2. Theory

Equations of state are accurate tools for predicting and modelling the thermodynamic properties of materials over a wide range of temperatures and pressures. Not only can these equations model the properties of all forms of pure materials, including solids, liquids and gases, but also they can predict mixtures, surface and transport properties [9–11]. One of the oldest equations of state, which is based on theoretical studies and statistical mechanics, is the virial equation of state (VEOS), which has been used extensively to study the thermodynamic properties of gases.

$$Z = 1 + \sum_{n=2} B_n^+ P^{n-1}$$

or

$$Z = 1 + \sum_{n=2} B_n \rho^{n-1} \quad (1)$$

in which

$$\begin{aligned} B_2^+ &= B_2/RT \\ B_3^+ &= (B_3 - B_2^2)/R^2T^2 \end{aligned} \quad (2)$$

and it is better to consider $B_2 \equiv B$ and $B_3 \equiv C$. In the aforementioned equations, Z is the compressibility factor ($Z = pV_m/RT$), ρ is the density ($\rho = 1/V_m$) and B_n is the n th virial coefficient. As can be seen, at very

low pressures or densities, the compressibility factor is equal to one, and this is the ideal gas equation, $Z = 1$. Therefore, VEOS clearly shows the deviation from the ideal state. Based on statistical thermodynamic studies, it can be proved that the virial coefficients are related to intermolecular interactions. For example, the second coefficient B indicates the interaction between the pair of molecules as follows:

$$B(T) = -2\pi \int_0^\infty \left[e^{-u(r)/KT} - 1 \right] r^2 dr, \quad (3)$$

where $u(r)$ is the intermolecular interaction energy function. It is clear that when $u(r) \leq 0$, then $B \leq 0$. In the same way, the third coefficient $C(T)$ is the interaction of the three molecules, the fourth coefficient $D(T)$ is the interaction of the four molecules in the cluster, and so on. Since the virial coefficients depend on the intermolecular potentials, if no interaction occurs between the molecules, the virial coefficients will all be zero and because of this, VEOS shows the non-ideal behaviour of real fluids. So, virial coefficients together with virial equation of state (VEOS) are the connection bridge between microscopic and macroscopic properties and show non-ideality. From this point of view, by precisely determining the virial coefficients and using the virial equation, the thermophysical properties of fluids can be predicted and modelled with good accuracy.

It has been shown that virial coefficients can be obtained using various theoretical and experimental methods with very good accuracy [12–24]. Examples of experimental methods are speed of sound and Joule–Thomson measurements and examples of theoretical methods are the use of EOS and interaction potential functions.

Due to the importance and existence of two-molecule and three-molecule interactions in the fluid, many types of research have been done by different researchers to determine these coefficients accurately and some of them provide accurate correlation equations for many molecules, for example alkanes and their mixtures [25–44]. In this respect, a correlation function of the second virial coefficient for C_2H_4 and CH_4 had been presented by Boushehri *et al* [45]. Also, Zarkova *et al* presented second *PVT*–virial coefficients $B(T)$ for 11 heavy globular gases in 2002 [46] and pure small alkanes CH_4 to $n\text{-C}_5\text{H}_{12}$ in 2006 [47].

VEOS is the equation of state that can be used for calculating and modelling the thermodynamic properties of fluids. In that equation, third terms onwards can be ignored at low pressure or density and finally

$$\begin{aligned} Z &= 1 + B\rho \\ \text{or} \\ Z &= 1 + B^+P. \end{aligned} \quad (4)$$

As mentioned earlier, by having accurate virial coefficients and using VEOS, the thermophysical properties of fluids can be predicted with good accuracy. In our previous papers [49,50], we obtained equations to model the thermodynamic behaviours of some refrigerants and SF₆ and showed that this approach can predict the mentioned behaviours. In this paper, we are going to present the estimation and modelling of some thermodynamic properties of small alkanes using Zarkova’s correlation equation to evaluate it. This correlation for the second virial coefficient is as follows:

$$B(T) = d_1 + \frac{d_2}{T} + \frac{d_3}{T^2} + \frac{d_4}{T^3} = \sum_{n=1}^4 \frac{d_n}{T^{n-1}} \quad (5)$$

in which d_n are expansion coefficients of the equation and tabulated in table 1.

In this work, some thermodynamic properties of CH₄ to n -C₅H₁₂ at low pressure are calculated and modelled using eqs (4) and (5).

3. Thermophysical properties

In this work, the following thermodynamic properties of the aforementioned molecules are estimated and modelled.

3.1 Joule–Thomson coefficient

The Joule–Thomson (JT) effect is related to the change in temperature that occurs when a gas expands through a porous plug into a region of lower pressure. For most of the real gases, the temperature falls under these circumstances as the gas has to do internal work to overcome the intermolecular forces for the expansion to take place. At ordinary temperature and pressure, all real gases undergo expansion and this phenomenon is used in the process of liquefying gases. JT effect is most widely used in refrigeration and gas liquefaction processes. μ_{JT} is the Joule–Thomson coefficient and is defined as

$$\mu_{JT} = \left(\frac{\partial T}{\partial P} \right)_H = -\frac{1}{C_{P,m}} \left(\frac{\partial H}{\partial P} \right)_T, \quad (6)$$

where $C_{P,m}$ is the molar heat capacity. This coefficient can be positive, negative or zero. μ_{JT} can be shown as the expansion by pressure in which expansion coefficients depend on virial coefficients [48,49]

$$\mu_{JT} = \frac{1}{C_{P,m}} \sum_{n=0} A_n P^n = \frac{1}{C_{P,m}} (A_0 + A_1 P + \dots)$$

$$A_0 = T \frac{dB}{dT} - B$$

$$A_1 = \frac{1}{R} \left(\frac{dC}{dT} - 2B \frac{dB}{dT} \right) + \frac{2}{RT} (B^2 - C). \quad (7)$$

At zero pressure, we have

$$\mu_{JT}^0(T) = \frac{A_0(T)}{C_{P,m}^0} = \frac{1}{C_{P,m}^0} \left(T \frac{dB(T)}{dT} - B(T) \right)$$

$$A_0(T) = \mu_{JT}^0(T) C_{P,m}^0(T) = - \left(\frac{\partial H}{\partial P} \right)_T^0 \quad (8)$$

in which μ_{JT}^0 , $C_{P,m}^0$ and $(\partial H/\partial P)_T^0$ are JT coefficient, heat capacity and the enthalpy changes at zero pressure or at ideal conditions respectively. In my previous papers, it was shown that μ_{JT}^0 can be written as follows [49,50]:

$$\mu_{JT}^0(T) = \frac{1}{(1 + \frac{3}{2}N)R} \left(T \frac{dB(T)}{dT} - B(T) \right) \quad (9)$$

in which, N is the number of atoms in the molecule. Since no interaction occurs between the molecules of an ideal gas, its JT coefficient is zero. But as shown in eqs (7) and (9), μ_{JT}^0 of real gas will not be zero even at zero pressure. Hence, the JT coefficient at zero pressure of a real gas can be considered as the rate of deviation of that gas from the ideal state due to two molecular interactions.

3.2 Deviation function

Deviation functions in thermodynamics represent the amount of deviation of fluids at different temperatures and pressures from the ideal state. For the deviation function of enthalpy on the thermodynamic relations, we have

$$H_m^{id}(T, P) - H_m(T, P) = \int_0^P \left[T \left(\frac{\partial V_m}{\partial T} \right)_P - V_m \right] dP. \quad (10)$$

This deviation, the same as μ_{JT}^0 , can be written as the expansion by pressure in which expansion coefficients depend on virial coefficients as follows [48–50]:

$$H_m^{id}(T, P) - H_m(T, P) = \sum_{n=1} b_n P^n$$

$$b_1 = A_0 = T \frac{dB}{dT} - B$$

$$b_2 = \frac{1}{2} A_1 = \frac{1}{2R} \left(\frac{dC}{dT} - 2B \frac{dB}{dT} \right) + \frac{1}{RT} (B^2 - C). \quad (11)$$

Therefore, non-ideality measurement can be done using virial coefficients. It is clear that the deviation function of enthalpy is equal to zero when $P = 0$ and

Table 1. Coefficients of correlation equation.

Molecule	d_1	d_2	d_3	d_4
CH ₄	46.515	–20175.6	–1706960	–61767800
C ₂ H ₆	106.351	–77035.3	1673500	–1365630000
C ₃ H ₈	180.925	–155269	12013700	–4990880000
C ₄ H ₁₀	324.441	–322979	57562600	–15858100000
C ₅ H ₁₂	585.369	–731564	230020000	–49473100000

of course, at low pressure, second terms onwards can be ignored in the expansion.

3.3 Fugacity coefficient

Fugacity is a measure of the real pressure or pressure of a gas in comparison to an ideal gas. In thermodynamics, the fugacity of a real gas is an effective partial pressure that replaces the mechanical partial pressure. Fugacity is determined experimentally or estimated from various models. The real gas pressure and fugacity are related through the dimensionless fugacity coefficient φ

$$\frac{f}{P} = \varphi. \quad (12)$$

For an ideal gas, fugacity and pressure are equal and so $\varphi = 1$. φ can be calculated as

$$\ln \varphi = \int_0^P \left(\frac{Z - 1}{p} \right) dp \quad (13)$$

in which Z can be obtained from EOS. Using eqs (1) and (13), $\ln \varphi$ can be written as the expansion by pressure in which expansion coefficients depend on virial coefficients as follows:

$$\begin{aligned} \ln \varphi &= \sum_{n=1} C_n P^n \\ C_1 &= \frac{B}{RT} P \\ C_2 &= \frac{1}{2R^2 T^2} (C - B^2). \end{aligned} \quad (14)$$

As seen, $\varphi = 1$ when $P = 0$. Like earlier, second terms onwards can be ignored in the expansion.

3.4 Thermal expansion

Thermal expansion is a material property that is indicative of the extent to which a material expands upon heating. Different substances expand by different amounts. The volumetric coefficient of thermal expansion is given by

$$\alpha = \frac{1}{V_m} \left(\frac{\partial V_m}{\partial T} \right)_p. \quad (15)$$

It can be shown that thermal expansion depends on the virial coefficient. At low pressure, we have

$$\alpha = \frac{1}{V_m} \left(\frac{R}{P} + \frac{dB}{dT} \right). \quad (16)$$

As can be seen, the coefficient of thermal expansion is a function of the slope of the changes of the second virial coefficient with respect to temperature. It is clear that the increase or decrease of intermolecular interactions due to temperature changes affects the thermal expansion of fluids.

3.5 Bulk modulus

Bulk modulus is a thermodynamic property of the fluids

$$\beta_T = \rho \left(\frac{\partial P}{\partial \rho} \right)_T. \quad (17)$$

Given that virial equation, bulk modulus can be written as follows at low pressure:

$$\beta = RT(\rho + 2B\rho^2). \quad (18)$$

It is clear that with increasing intermolecular interactions, bulk modulus also increases.

4. Results and discussion

In this work, the thermodynamic properties of small alkanes are calculated and modelled by Zarkova's correlation function of the second virial coefficient and VEOS.

The results of the second virial coefficient of the studied molecules can be used to evaluate the strength of their intermolecular interactions and to compare them with each other from this viewpoint. As told before, the second virial coefficient depends on intermolecular interaction potential energy, so that with increasing intermolecular attractive forces, the second virial coefficient decreases and the Boyle temperature increases.

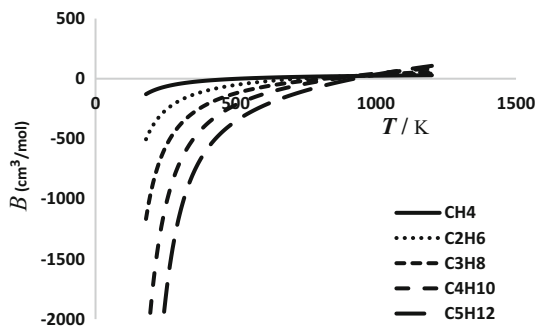


Figure 1. Second virial coefficients of the studied molecules as a function of temperature.

As can be seen in figure 1, at a given temperature below the Boyle temperature, the value of the second virial coefficient of the studied molecules in comparison with each other is of the order $C_5H_{12} < C_4H_{10} < C_3H_8 < C_2H_6 < CH_4$ and table 2 also shows that the order of Boyle temperature increase is $T_B(CH_4) < T_B(C_2H_6) < T_B(C_3H_8) < T_B(C_4H_{10}) < T_B(C_5H_{12})$. Therefore, C_5H_{12} has the strongest interaction and CH_4 has the lowest one among the molecules studied.

Since the Boyle temperature (T_B) and Boyle volume (V_B) were found to be sensitive to the equation in use [51], we determined them using the correlation equation and compared them with other sources [27,52]. Boyle temperature (T_B) is the temperature at which $B(T_B) = 0$ and the Boyle volume (V_B) can be obtained as follows:

$$V_B = T_B \left(\frac{\partial B}{\partial T} \right)_{T=T_B} \quad (19)$$

At this temperature and volume, attractive and repulsive forces are equal and the fluid behaves like an ideal gas. The results are shown in table 2.

Table 2. Calculated Boyle temperature (T_B) and Boyle volume (V_B) of the studied molecules.

Molecule	T_B		V_B
	This work	Source	
CH ₄	510.69	510.39 [44]	53.98
		503.26 [45]	
C ₂ H ₆	727.0	757.52 [44]	110.29
		770.15 [45]	
C ₃ H ₈	818.24	880.03 [44]	181.2
		908.10 [45]	
C ₄ H ₁₀	854.83	976.45 [44]	296.44
		1019.23 [45]	
C ₅ H ₁₂	923.29	1040.84 [44]	441.25
		1097.94 [45]	

μ_{JT}^0 of the studied alkanes are shown in figure 2. As can be seen, with decreasing temperature, μ_{JT}^0 increases sharply, and with increasing temperature, this coefficient goes to zero. This behaviour is predicted very well qualitatively in a wide range of temperature.

In figure 3, variations of molar volume of CH_4 and C_3H_8 in terms of temperature at $P = 1$ atm is shown and compared with experimental data [53]. As can be

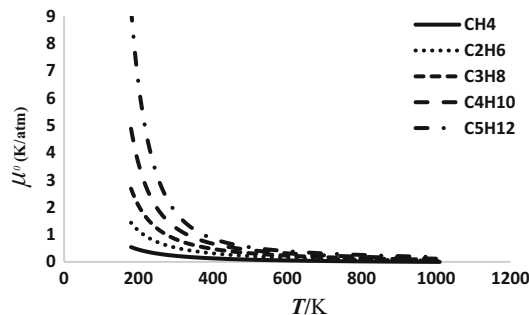


Figure 2. The calculated zero-pressure Joule–Thomson coefficient of small alkanes vs. temperature.

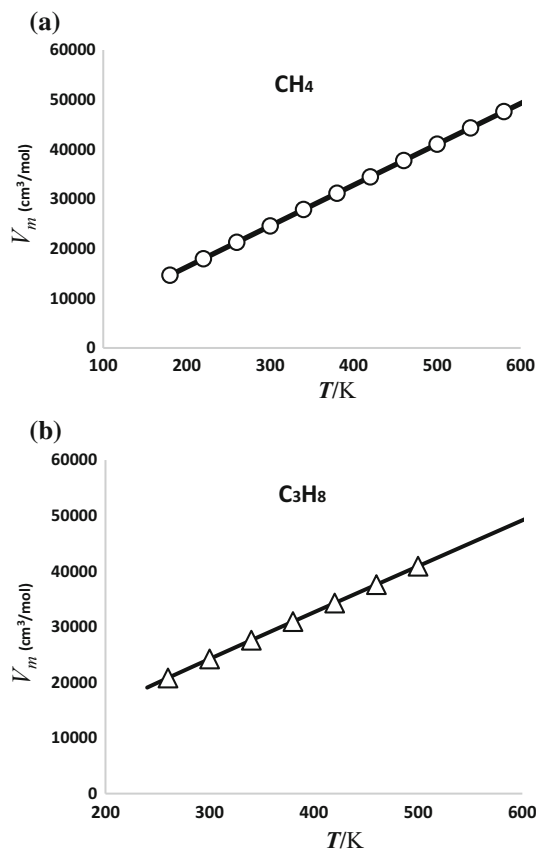


Figure 3. Variations of molar volume of (a) CH_4 and (b) C_3H_8 in terms of temperature at $P = 1$ atm. The line indicates this work and the triangles indicate experimental data.

seen, the correlation equations predict this behaviour for the studied molecules very well qualitatively and quantitatively.

In figures 4 and 5, A^0 and $H_m^{id} - H_m$ of the aforementioned molecules are compared with each other and experimental data [53]. As can be seen, there is an excellent agreement between experimental and theoretical results. Meanwhile, it is clear that due to the stronger interaction in C_5H_{12} than in others, this molecule shows more deviation than the others.

Figure 6 shows variations of fugacity coefficient of methane and ethane vs. temperature at pressures 0.5 and 1.0 atm and the results have been compared with experimental data [53]. It is clear that, $\ln \phi$ goes to zero with increasing temperature and decreases with increasing pressure because of the increasing intermolecular forces. The model presented qualitatively and quantitatively predicts this behaviour very well. In this respect, figure 7 shows variations of fugacity coefficient of all the studied molecules as a function of temperature compared to each other and experimental data [53] and as

can be seen, there is an excellent agreement between experimental and theoretical results. It is clear that due to the stronger interaction in C_5H_{12} , this molecule shows more deviation than the other molecules and the ideal state.

Figures 8a and 8b respectively show the behaviour of thermal expansion of propane and butane in terms of

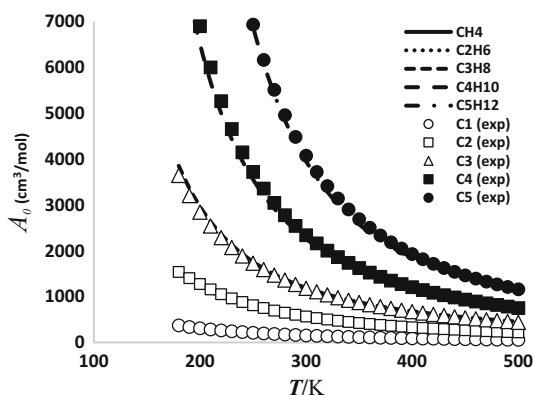


Figure 4. The calculated $A_0 = -(\partial H/\partial P)_T^0$ of the studied molecules as a function of temperature.

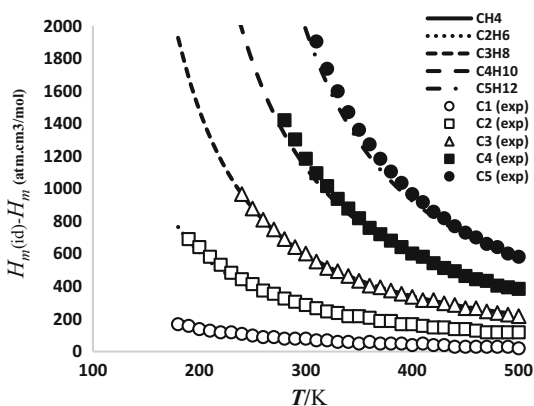


Figure 5. Deviation function of enthalpy of the studied molecules as a function of temperature.

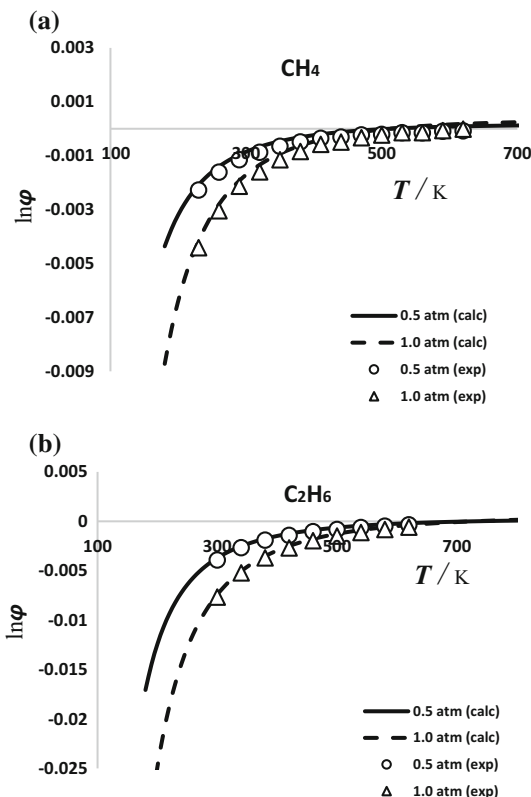


Figure 6. Variations of fugacity coefficient of (a) CH_4 and (b) C_2H_6 vs. temperature.

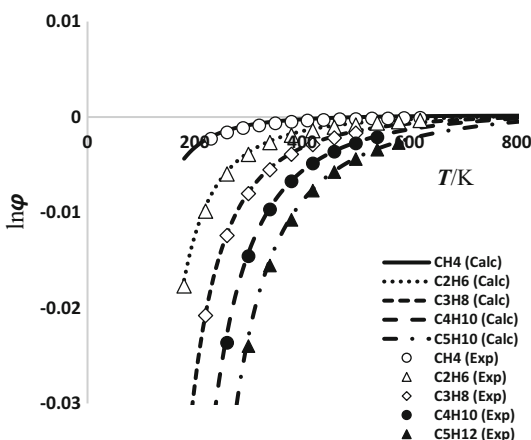


Figure 7. Variations of fugacity coefficient of the studied molecules in terms of temperature.

temperature compared with experimental data [53]. This behaviour is qualitatively and quantitatively predicted and modelled very well, by the correlation equation. This property for all molecules studied is shown in figure 9 and compared with each other and the experimental study. The agreement between theoretical and experimental results is excellent.

The curve of isothermal bulk modulus for CH₄ and C₅H₁₂ as a function of pressure calculated by correlation equation is shown in figure 10 and compared with experimental data [53]. As seen, the curve is completely linear. Linear behaviour of the bulk modulus vs. pressure is one of the thermodynamic regularity of materials. Based on this regularity, the bulk modulus of the fluid is nearly linear in pressure for each isotherm [54,55]

$$B_T = B_{0,T} + B'_{0,T} P, \tag{20}$$

where $B_{0,T}$ is B_T in zero pressure and $B'_{0,T}$ is the slope of the bulk modulus at zero pressure. $B_{0,T}$ and $B'_{0,T}$ are temperature-dependent parameters. This regularity was

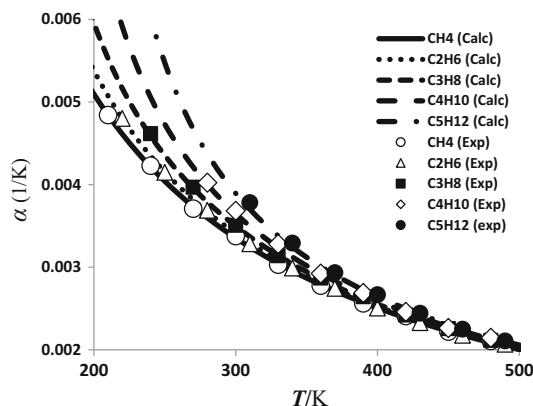


Figure 9. Variations of thermal expansion of the studied molecules vs. temperature.

first noticed by P G Tait over 100 years ago and is now called the Tait–Murnaghan regularity. This regularity is predicted qualitatively and quantitatively very well, by the correlation equation.

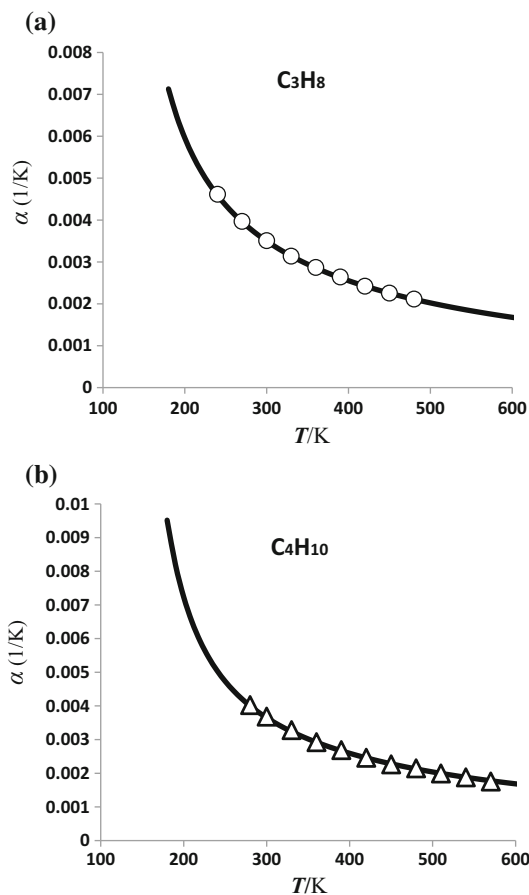


Figure 8. Variations of thermal expansion of (a) C₃H₈ and (b) C₄H₁₀ vs. temperature. The line indicates this work and the triangles indicate the experimental data.

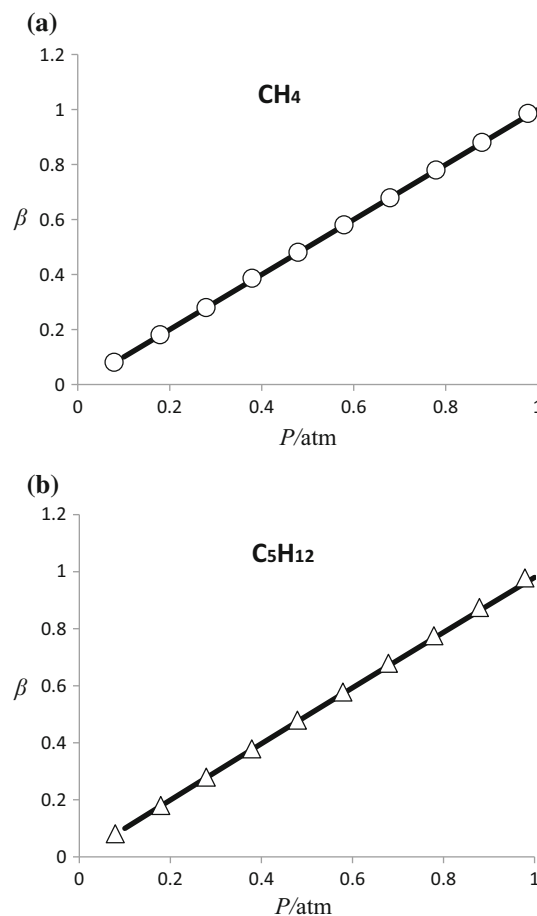


Figure 10. The behaviour of the bulk modulus of (a) CH₄ and (b) C₅H₁₂ vs. pressure. The line indicates this work and the triangles indicate the experimental data.

5. Conclusion

In this work, some thermodynamic properties of small alkanes at low pressure and wide range of temperature were calculated and modelled to evaluate the performance of Zarkova's correlation equation of the second virial coefficient. For this purpose, five materials, CH₄, C₂H₆, C₃H₈, *n*-C₄H₁₀ and *n*-C₅H₁₂, were selected and studied. In addition, Boyle temperature and Boyle volume were also calculated. The obtained results show that thermodynamic properties of the studied materials and their deviation from the ideal state have been predicted and modelled very well by the correlation equation presented in a wide range of temperatures.

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