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CALCULATION of COMPRESIBILITY COEFFICIENT using THIRD VIRIAL COEFFICIENT over KIHARA POTENTIAL

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Abstract – Kihara potential has used to calculate the thermodynamic properties of complex real gases. In this study, the numeric method has been suggested for calculating compressibility coefficient using the third virial coefficient over Kihara potential. The accuracy of the numeric method has been tested by application to gas CH_4. It was seen in this work that the obtained results for compressibility coefficient for CH_4 are approximately agreement with the literature. It was seen that it gave results close to the literature in wide pressure and temperature ranges.

Keywords – Third Virial Coefficient, Kihara Potential, Compressibility Coefficient

INTRODUCTION

The thermodynamic properties of imperfect gases have been investigated with theoretically and experimentally methods [1-5]. Many authors have been offered to theoretical method defined the thermodynamic properties of imperfect gases [6-8]. The virial equation state is one of these methods. The thermodynamic properties of imperfect gases can be calculated accurately and precisely in certain temperature and pressure ranges [8]. Here, the intermolecular interaction potentials are very important to calculate according to virial coefficients. Therefore, intermolecular interaction potentials, which are selected according to the structure of the molecule, are Lennard-Jones (12-6), Kihara, Yukawa, and Stockmayer potentials, etc [9]. The advantage of Kihara potential is a better defined of the thermodynamic and transport properties of complex fluids [10,12].

In this work, the compressibility coefficient of CH_4 was calculated by using the third virial coefficient over Kihara potential, in different temperature and pressure ranges. The results obtained were compared with available other method in the literature.

MATERIALS AND METHODS

The third virial coefficient is defined in the following form [8]

$$C(T) = -\frac{N_A^2}{3}\iiint f(r_{12})\, f(r_{13})\, f(r_{23})\, dr_{12} dr_{13} \quad . \tag{1}$$

Here, $f(r_{ij}) = exp\left(u(r_{ij})/k_B T\right) - 1$ is Mayer functions and N_A is Avogadro's constant. In Mayer function,

$u\left(r_{ij}\right)$ is the intermolecular potential, T is temperature and k_B is the Boltzmann constant [8].

Table 1. Results of calculation compressibility coefficient of CH_4

$P(atm)$	$T(K)$	Z	Z Ref. [13]
0.1	200	1.0000000001831497	0.9994
	300	1.0000000000321014	0.9998
	400	1.0000000000092646	1
	500	1.0000000000034577	1
1	200	1.000000018314978	0.9936
	300	1.0000000032101384	0.9983
	400	1.0000000009264478	0.9995
	500	1.0000000003457592	1
3	200	1.000000164834801	0.9806
	300	1.000000028891245	0.9949
	400	1.0000000083380305	0.9986
	500	1.000000003111832	0.9999
5	200	1.0000004578744468	0.9675
	300	1.0000000802534583	0.9915
	400	1.0000000231611959	0.9977
	500	1.0000000086439775	0.9999

In the previous work, for evaluating of the third virial coefficient, we presented numeric method following form [11]:

$$C^*\left(T^*\right)=\frac{6}{\left(1+a^*\right)^6}\left[\int_0^\infty\left(e^{-\frac{4}{T^*}\left(\left(r_{12}^*-a^*\right)^{-12}-\left(r_{12}^*-a^*\right)^{-6}\right)}-1\right)\int_0^\infty\left(e^{-\frac{4}{T^*}\left(\left(r_{13}^*-a^*\right)^{-12}-\left(r_{13}^*-a^*\right)^{-6}\right)}-1\right)\int_{-1}^{1}\left(e^{-\frac{4}{T^*}\left(\left(\sqrt{r_{12}^2+r_{13}^2-2r_{12}r_{13}\eta}-a^*\right)^{-12}-\left(\sqrt{r_{12}^2+r_{13}^2-2r_{12}r_{13}\eta}-a^*\right)^{-6}\right)}-1\right)r_{12}^{*2}r_{13}^{*2}d\eta dr_{12}dr_{13}\right] \quad (2)$$

where, $C^*\left(T^*\right)=C\left(T^*\right)/b_0^2$, $b_0=2\pi N_A\sigma^3/3$, $r_{ij}/\sigma-2a=r_{ij}^*$, $a/\sigma-2a=a^*$ and $T^*=k_BT/\varepsilon$ [11].

The Kihara potential in Eq. (2) [9]:

$$u(r)=\begin{cases}\infty & r<2a\\ 4\varepsilon\left(\left(\frac{\sigma-2a}{r-2a}\right)^{12}-\left(\frac{\sigma-2a}{r-2a}\right)^{6}\right) & r\geq 2a\end{cases} \quad (3)$$

,

The substituting Eq. (2) into the Eq. (4), we have calculated compressibility coefficient. The compressibility coefficient is written following as:

$$Z=\frac{PV}{RT}=1+C(T)\left(\frac{P}{RT}\right)^2 \quad (4)$$

where P is pressure, R is universal gas constant, T is temperature and C(T) is third virial coefficient [8]. The compressibility coefficient calculation results obtained at different temperature and pressure ranges are given in Table 1.

NUMERICAL RESULTS and DISCUSSION

In this paper, we have presented numeric method for compressibility coefficient using third virial coefficient over Kihara potential. The suggested numeric method is general and free of any restriction on its applications to complex real gases. Numerical calculations for compressibility coefficient of CH_4 have performed using Mathematica 7.0 Software program. The obtained results are compared with available literature data [13] and it shows approximately agreement in the literature data.

The obtained results of the compressibility coefficient of CH_4 are given in Table 1. As can be seen in Table 1, the results are approximately good agreement with literature data. In consequence, the certain temperature and pressure range of the used numeric method offers the advantage of the correct calculation of the compressibility coefficient with the third virial coefficient.

CONCLUSION

A numeric method for evaluating thermodynamic properties of imperfect gases is presented, in his work. The accuracy and precision of results demonstrate that the suggested numeric method is

applicable to imperfect gases at a certain range of temperatures for compressibility coefficient.

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