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## Modeling some thermodynamic properties of UF<sub>6</sub> at low pressure using correlation function

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### ABSTRACT

The properties of uranium hexafluoride (UF<sub>6</sub>) are very important to the nuclear industry as a precursor for its enrichment. Therefore, it is significant to obtain the most accurate properties for this strategic compound. In this paper, some thermophysical properties of uranium hexafluoride (UF<sub>6</sub>) at low pressure and below the critical temperature are predicted. Also, by using its correlation function to the second virial coefficient and virial equation of state (VEOS) it is being modeled. The studied properties consisted of Joule-Thomson coefficient, enthalpy, deviation function, fugacity coefficient, thermal expansion, and isothermal compressibility. So far, several researchers have studied virial coefficients of UF<sub>6</sub>, and some of them have presented its correlation function of the second virial coefficient. In this paper, the studied correlation functions are the ones suggested by Dymond and Zarkova. The obtained results show that the correlation equations presented have a good ability to predict and model the thermophysical properties of uranium hexafluoride. Moreover, its deviation from the ideal state especially in the temperature range from 360 K up to critical temperature is satisfactory.

**Keywords:** Uranium hexafluoride; Virial coefficients; Correlation function; Thermodynamic properties

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### I. INTRODUCTION

Uranium hexafluoride (UF<sub>6</sub>) is a material used principally in the production of nuclear fuels. It is a colorless subliming solid. It was first prepared by Ruff (in 1909) who described it as a pale yellow, very reactive substance, and a strong fluorinating agent. The leakage of UF<sub>6</sub> into the environment and chemical reaction with water vapor would result in the formation of highly toxic UO<sub>2</sub>F<sub>2</sub> aerosols and gaseous hydrofluoric acid (HF) [1]. The sublimation point at atmospheric pressure is at

56.2 °C, while melting occurs in the range 64.5-64.8 °C with the triple point at  $T= 64.02$  °C and  $P= 1.497$  atm [1-2]. Since this work is mainly related to the pressures below 1 atm, the discussion of the critical point ( $T= 230.2$  °K and  $P= 45.5$  atm) will be beyond this paper. The properties of uranium hexafluoride (UF<sub>6</sub>) are important for the nuclear industry as a precursor to enrichment. It is therefore important to obtain the most accurate characteristics for such a strategic combination.

Not much information about the thermophysical properties of  $UF_6$  is available in the sources [3]. There are few articles in this field. This is probably due to experimental problems in preparing and working with samples of pure materials, which are very corrosive due to the presence of moisture and fluorination of many materials [2-5]. Unfortunately, the data in the articles on the thermophysical properties and coexistence of  $UF_6$  phases are inconsistent. This is especially true of the vapor-liquid properties. The problem is for an almost super-critical region in which experimental data are practically non-existent [2-3]. As a result, there is a need for the ability to model the phase behavior and thermophysical properties of  $UF_6$ . Joule-Thomson [6] calculated the deviation functions for refrigerant fluids in order to evaluate the performance of their correlation equation at low pressure and a wide range of temperatures, in his previous paper. The results showed that the accurate correlation equation presented had a very good ability to predict the thermophysical properties of materials and their deviation from the ideal state over a wide range of temperatures. In this paper, we calculate and model some thermodynamic properties of  $UF_6$  at low pressure using its virial coefficients and virial equation of state (VEOS). This approach has not been used to calculate and model some of the thermophysical properties of this material, so far.

## II. VIRIAL EQUATION OF STATE (VEOS)

One of the important tools for the correlation and prediction of the thermodynamic properties of gases, liquids, and even solids over a wide range of temperatures and pressures is the Equation of State (EOS). Since it is a powerful tool for determining the data required, many publications used it for their development [7-9]. One of the oldest models for calculating the thermophysical properties of

fluids is the virial equation of state (VEOS), which provides the required information with relatively good accuracy.

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

or

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

$$B_2^+ = B_2 / RT,$$

$$B_3^+ = (B_3 - B_2^2) / R^2 T^2,$$

$$B_2 \equiv B \text{ and } B_3 \equiv C,$$

where  $Z$  is the compressibility factor ( $Z = PV_m / RT$ ),  $\rho$  is the density ( $\rho = 1 / V_m$ ), and  $B_n$  is  $n$ th-virial coefficient. It is clear that when the pressure or density becomes zero, the compressibility factor will be one, and this is the ideal gas equation,  $Z = 1$ . Therefore, the virial equation shows the deviation from the ideal state. The fundamental fact about VEOS is that it has a strong theoretical basis in statistical mechanics. In fact, the virial coefficients are related to intermolecular interactions by exact statistical-mechanical formulae. In this respect,  $n$ th-virial coefficient is related to molecular interactions in clusters of  $n$  molecules. For example, the second coefficient  $B$  indicates the interaction between the pair of molecules as follows:

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

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  $C$  to the interaction of the three molecules in the cluster, and so on. Thus, the virial coefficients are the connection bridge between microscopic and macroscopic properties and show the non-ideal behavior of real fluids [10]. From this viewpoint,

by accurately identifying the virial coefficients and how they depend on temperature and using VEOS, it can be easy to calculate and model the thermodynamic properties of fluids. Virial coefficients can be obtained using both experimental and theoretical methods [11-23]. Experimental methods consist of *PVT* measurements, speed of sound measurements, Joule–Thomson measurements, refractive index and relative permittivity measurements and vapor pressure, and enthalpy of vaporization measurements. Theoretical approaches usually consist of using equations of state and interaction potential functions. Most of the research on virial coefficients is related to the second and third coefficients, and attempts are made to obtain a general correlation relationship for many molecules. In 1957, for the second virial coefficients of nonpolar gases, Pitzer and Curl [24] presented a successful correlation. Then this correlation has been modified by O’Connell and Prausnitz [25], Tsonopoulos [26-27], Tarakad and Danner [28], Orbey [29], Weber [30], and Hayden and O’Connell [22] using refitting the coefficients of the Pitzer–Curl correlation, added polar and hydrogen bonding terms and applied new parameters. In 1987, Boushehri presented a correlation function of the second virial coefficient for the linear molecules like  $N_2$ , near-linear molecules like  $C_2H_4$ , and near-spherical molecules like  $CH_4$  [31].

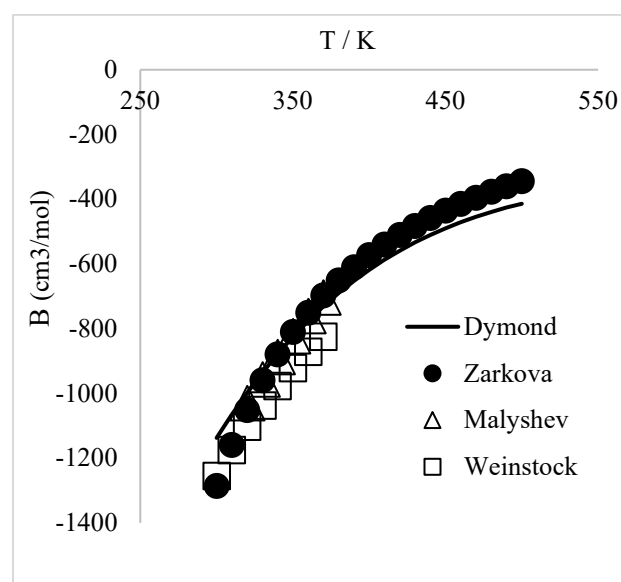
So far, several researchers have studied virial coefficients of  $UF_6$  and some of them have presented its correlation function of the second virial coefficient [32-39]. Some of the important ones consist of Weinstock in 1959 [32], Dewitt in 1960 [33], Malyshev in 1973 [34], Dymond [37] and Zarkova [38] in 2002. These correlations are in the form of the following equation:

$$B(T) = a_1 + \frac{a_2}{T} + \frac{a_3}{T^2} + \frac{a_4}{T^3} = \sum_{n=1}^4 \frac{a_n}{T^{n-1}}, \quad (3)$$

in which the expansion coefficients of equation ( $a_n$ ) are tabulated in Table 1.

In this respect, Figure 1 compares the four of these correlation functions. As can be seen, except Weinstock correlation, there is a good match between them in the temperature range  $350 < T < 500$  K. Since these correlation functions have been obtained by fitting experimental data, therefore it can be considered that the second virial coefficient of  $UF_6$  in that range of temperature  $350 < T < 500$  K is completely matched with experimental data.

In this paper, the thermophysical properties of  $UF_6$  are modeled from 350 K to its critical temperature. Characterization modeling is the use of VEOS at low pressure and the second virial coefficient of which is obtained from Zarkova and Dymond’s correlation equations. The use of virial coefficients to model some of the thermophysical properties of  $UF_6$ , which is the subject of this research, has not been done before.



**Fig. 1.** Correlation function of second virial coefficient in various models

**Table 1**  
The Expansion Coefficients of the Equation (2) in Various Models of Correlation

B (cm <sup>3</sup> /mol) (correlation model)	Temperature range (K)	$a_1$	$a_2$	$a_3$	$a_4$
Zarkova	200-900	1033	$-1.46 \times 10^6$	$6.2 \times 10^8$	$-1.172 \times 10^{11}$
Dymond	300-470	- 1697.7	$1.8712 \times 10^6$	$-7.7035 \times 10^8$	$7.7828 \times 10^{10}$
Malyshev	320-370	3.94	2197	0	0
Weinstock	270-370	0	0	$1.12974 \times 10^8$	0

At low pressure or density, the third terms of virial equation of state (VEOS) onwards can be ignored in the expansion and we have:

$$Z = 1 + B\rho,$$

or

$$Z = 1 + B^+P. \quad (4)$$

Therefore, using Equation (4) and having only the second virial coefficient, many thermodynamic properties of fluids can be predicted and modeled. In this regard, we have:

$$Z_{Zarkova} = 1 + \left( 1033 - \frac{1.46 \times 10^6}{T} + \frac{6.2 \times 10^8}{T^2} - \frac{1.172 \times 10^{11}}{T^3} \right) \rho, \quad (5)$$

$$Z_{Dymond} = 1 + \left( -1697.7 + \frac{1.8712 \times 10^6}{T} - \frac{7.7035 \times 10^8}{T^2} + \frac{7.7828 \times 10^{10}}{T^3} \right) \rho. \quad (6)$$

In this work, some thermophysical properties of UF<sub>6</sub> at low pressure and below the critical temperature are calculated and modeled using Equations (5) and (6).

### III. THERMOPHYSICAL PROPERTIES

In our work, we calculate the following thermophysical properties of UF<sub>6</sub> using two correlation functions of the second virial coefficient.

#### A. Joule-Thomson Coefficient

In thermodynamics, the Joule-Thomson (J-T) effect is related to the temperature change of fluid when that fluid is forced to pass through a valve or porous plug so that heat is not exchanged with the environment. The J-T effect is of considerable importance in refrigeration and gas liquefaction processes. In this regard, the J-T coefficient ( $\mu_{JT}$ ) is defined as follows:

$$\mu_{JT} = \left( \frac{\partial T}{\partial P} \right)_H = -\frac{1}{C_{p,m}} \left( \frac{\partial H}{\partial P} \right)_T, \quad (7)$$

in which,  $C_{p,m}$  is heat capacity. This coefficient can be positive, negative, or zero. Joule-Thomson coefficient can be shown as the expansion by pressure in which expansion coefficients depend on virial coefficients as follows [6,39]:

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

$$A_0 = T \frac{dB}{dT} - B, \tag{8}$$

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

At zero pressure, we have

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

$$A_0(T) = \mu_{JT}^0(T) C_{P,m}^0(T) = - \left( \frac{\partial H}{\partial P} \right)_T^0, \tag{9}$$

where  $\mu_{JT}^0$  and  $C_{P,m}^0$  are Joule-Thomson coefficient and heat capacity at zero pressure, respectively. Also,  $(\partial H / \partial P)_T^0$  is the enthalpy changes relative to the pressure at zero pressure or at ideal conditions. In my previous paper, it was shown that zero pressure J-T coefficient can be written as follows [6]:

$$\mu_{JT}^0(T) = \frac{1}{\left(1 + \frac{3}{2} N\right) R} \left( T \frac{dB(T)}{dT} - B(T) \right), \tag{10}$$

where  $N$  is the number of atoms in molecule. Joule-Thomson coefficient of ideal gas is zero, because there is no interaction between their molecules. However, Equations (8) and (10) show that J-T coefficient of real gas is not zero in the limit of zero pressure. In this regard, zero pressure J-T coefficient ( $\mu_{JT}^0$ ) can be used as a measure of the deviation from the ideal state due to the interactions related to the pair of molecules [6,39]. These deviations can provide useful information about the nature of intermolecular forces.

### B. Deviation Function

As told before, the virial coefficients are the connection bridge between microscopic and macroscopic properties and show the non-ideal behavior of real fluids. Therefore, having virial coefficients, non-ideality measurement can be calculated using deviation functions in different pressures and temperatures. Based on the thermodynamic relations for deviation function of enthalpy, we have [39]:

$$H_m^{id}(T, P) - H_m(T, P) = \int_0^P \left[ T \left( \frac{\partial V_m}{\partial T} \right)_P - V_m \right] dP. \tag{11}$$

Deviation functions, the same as Joule-Thomson coefficient, can be written as the expansion of pressure in which expansion coefficients depend on virial coefficients as follows [6,39]:

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

$$b_1 = A_0 = T \frac{dB}{dT} - B, \tag{12}$$

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

It is clear that deviation functions are equal to zero when  $P = 0$  and of course, at low pressure, second terms onwards can be ignored in the expansion.

### C. Fugacity Coefficient

In chemical thermodynamics, the fugacity ( $f$ ) of a real gas is an effective partial pressure that replaces the mechanical partial pressure in an accurate computation of the chemical equilibrium constant. The real gas pressure and fugacity are related through the dimensionless fugacity coefficient  $\phi$

$$\frac{f}{P} = \phi. \tag{13}$$

For an ideal gas, the fugacity and pressure are equal and so  $\phi = 1$ . Taken at the same temperature and pressure, the difference between the molar Gibbs free energies of a real gas and the corresponding ideal gas is equal to  $RT \ln \phi$ . In this relation, the fugacity coefficient  $\phi$  can be calculated as:

$$\ln \phi = \int_0^p \left( \frac{Z-1}{p} \right) dp, \quad (14)$$

in which  $Z$  is compressibility factor that can be obtained from Equation of State. Using Equations (2) and (4), fugacity coefficient can be written as the expansion by pressure in which expansion coefficients depend on virial coefficients as follows:

$$\begin{aligned} \ln \phi &= \sum_{n=1} C_n P^n, \\ C_1 &= \frac{B}{RT} P, \\ C_2 &= \frac{1}{2R^2 T^2} (C - B^2). \end{aligned} \quad (15)$$

It is clear that the fugacity coefficient is equal to 1 when  $P=0$  and of course, at low pressure, second terms onwards can be ignored in the expansion.

#### D. Thermal Expansion

In the general case of a gas, liquid, or solid, the volumetric coefficient of thermal expansion is given by:

$$\alpha = \frac{1}{V_m} \left( \frac{\partial V_m}{\partial T} \right)_p, \quad (16)$$

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

$$\alpha = \frac{1}{V_m} \left( \frac{R}{P} + \frac{dB}{dT} \right). \quad (17)$$

#### E. Isothermal Compressibility

In classical thermodynamics, the isothermal compressibility is given by

$$\kappa = -\frac{1}{V_m} \left( \frac{\partial V_m}{\partial P} \right)_T, \quad (18)$$

that depends on virial coefficients. At low pressure we have:

$$\kappa = \frac{1}{RT(\rho + 2B\rho^2)}. \quad (19)$$

#### IV. RESULTS AND DISCUSSION

In this paper, some thermophysical properties of  $\text{UF}_6$  using two correlation equations were calculated. In Figure 2, variations of density of  $\text{UF}_6$  in terms of pressure at  $T=350$  K have been shown and compared with experimental data [40]. The experimental density of  $\text{UF}_6$  can be described according to an equation that is similar in form to the ideal gas law as follows [40]

$$\rho \text{ (Kg/m}^3\text{)} = \frac{4291 P}{T} \left( 1 + \frac{1.2328 \times 10^6 P}{T^3} \right). \quad (20)$$

As can be seen, the correlation equations predict this behavior very well qualitatively and quantitatively.

Figures 3 and 4 show the calculated zero pressure Joule-Thomson coefficient  $\mu_{JT}^0$  and enthalpy changes with respect to pressure  $A_0$  ( $= -(\partial H / \partial P)_T^0$ ) of  $\text{UF}_6$  as a function of temperature. As seen, with decreasing temperature both functions increase and with increasing temperature, the two go to zero. This fluid behavior is predicted very well by the two correlated

equations. It is also clear that the two correlations are exactly the same in the temperature range  $360 < T < 500$  K. It seems in that range, the change in  $\mu_{JT}^0$  and  $(\partial H / \partial P)_T^0$  as a function of temperature is linear and follows the equations:

$$\begin{aligned} \mu_{JT}^0 &= -0.0113 T + 6.5809, & 360 < T < 500 \text{ K} \\ (\partial H / \partial P)_T^0 &= 10.651 T - 6210.3. \end{aligned} \quad (21)$$

Figure 5 shows the calculated deviation function of enthalpy for  $\text{UF}_6$  versus temperature in different pressures 0.5 and 1.0 atm. As can be seen, with increasing temperature, the deviation decreases but it increases with increasing pressure. The same as before, the two correlations are the same in the range temperature  $360 < T < 500$  K.

As shown in Figures 3 to 5, the two curves below 350 K are quantitatively and qualitatively different. To explain this behavior, as mentioned earlier, the second virial coefficient depends on the potential energy of intermolecular interactions, so as the attractive molecular forces increase, the second virial coefficient decreases and following the Boyle temperature increases. As can be seen in Figure 1, at a given temperature below 350 K, the value of the second virial coefficient of two equations in comparison with each other is as  $B_{\text{Zarkova}} < B_{\text{Dymond}}$  and therefore according to the above,  $B_{\text{Zarkova}}$  shows more attractive force than the other. Because of this, thermodynamic properties calculated by Zarkove equation show greater deviation relative to the ideal conditions and exhibit greater J-T effect. This behavior can be clearly seen in Figures 6 and 7.

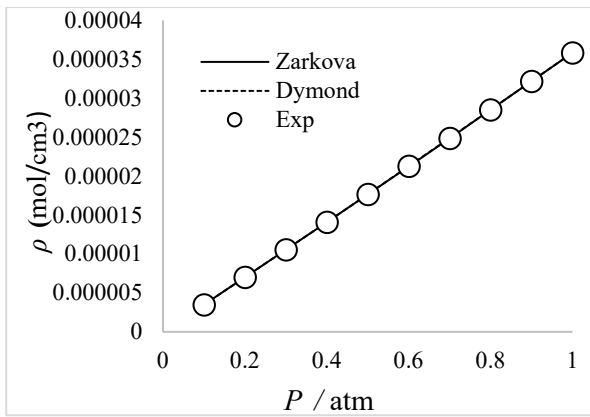
Variations of fugacity coefficient of  $\text{UF}_6$  as a function of temperature in pressures 0.5 atm are shown in Figure 6. It is clear that,  $\ln \phi$  goes to zero with increasing temperature and decreases with increasing the pressure because of increasing the

intermolecular forces. As known, with increasing temperature and decreasing pressure, the thermodynamic behavior of the gases goes to ideal gas conditions and therefore  $\phi=1$ , and  $\ln \phi \rightarrow 0$ . As observed, the correlation equations predict and model this behavior very well and are consistent with each other as before in the mentioned temperature range.

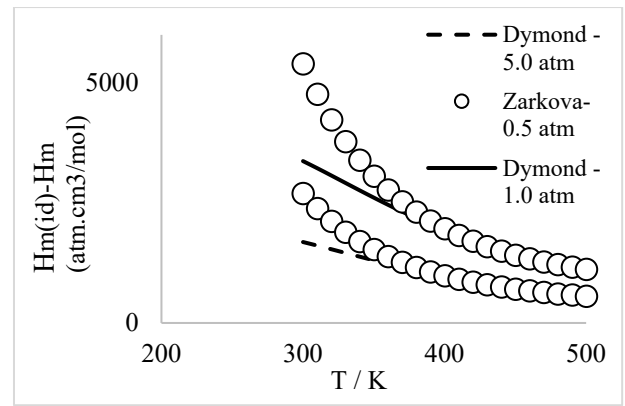
Figure 7 shows the behavior of the thermal expansion coefficient of  $\text{UF}_6$  vs temperature using Equation (17). As seen, this behavior is predicted well by correlation equations and the two present the same results completely. It is clear that as the temperature increases, the thermal expansion decreases, and from 500 K onwards, the thermal expansion behavior of  $\text{UF}_6$  is the same as that of the ideal gas due to what mentioned before.

The behavior of the isothermal compressibility of  $\text{UF}_6$  vs pressure is shown in Figure 8 using Equation (19). As seen, this behavior is predicted and modeled very well by correlation equations. It is clear that as the pressure increases,  $\kappa$  decreases and the two correlations are consistent with each other from zero to one atm pressure and are quite the same as that of the ideal gas quantitatively.

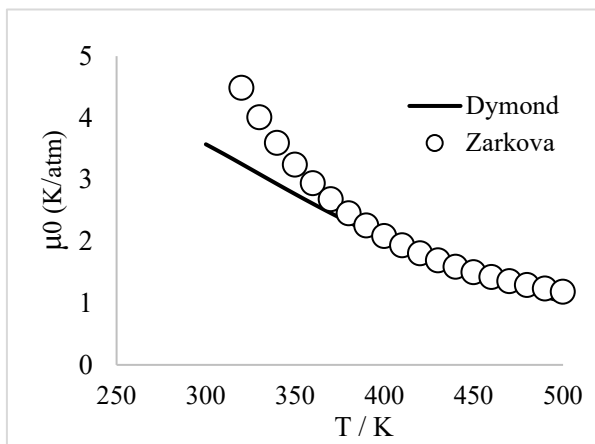
Due to the lack of experimental data available, the curves in Figures 3 to 8 have not been compared with the experimental results. However, since at a temperature range of 360 to 500 K, researchers have given the same results for the second virial coefficient of  $\text{UF}_6$ , so those data in that range can be considered accurate. Therefore, considering the results obtained from my previous article [6], the thermodynamic properties obtained in this way for  $\text{UF}_6$  can be considered in accordance with the experimental data.



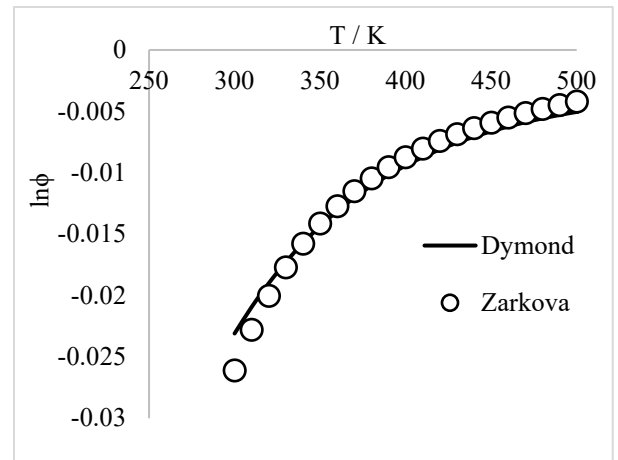
**Fig. 2.** Variations of density of  $UF_6$  in terms of pressure at  $T=350$  K



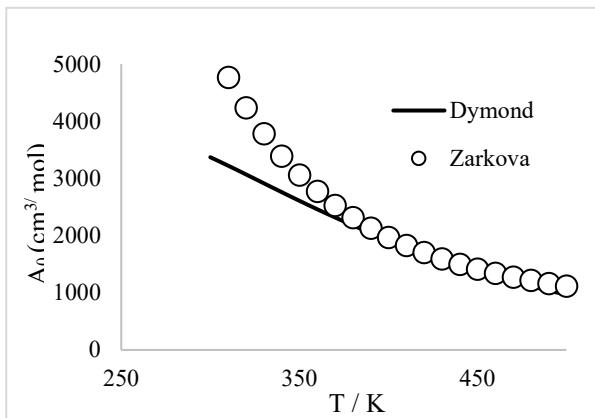
**Fig. 5.** Deviation function of enthalpy for  $UF_6$  in different pressures



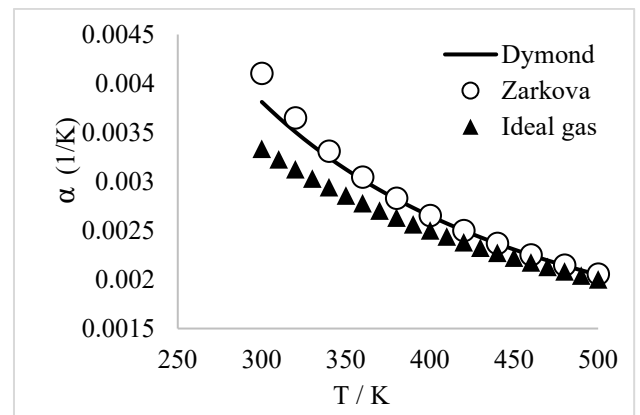
**Fig. 3.** The calculated zero pressure Joule Thomson coefficient of  $UF_6$  versus temperature



**Fig. 6.** Variations of fugacity coefficient of  $UF_6$  as a function of temperature

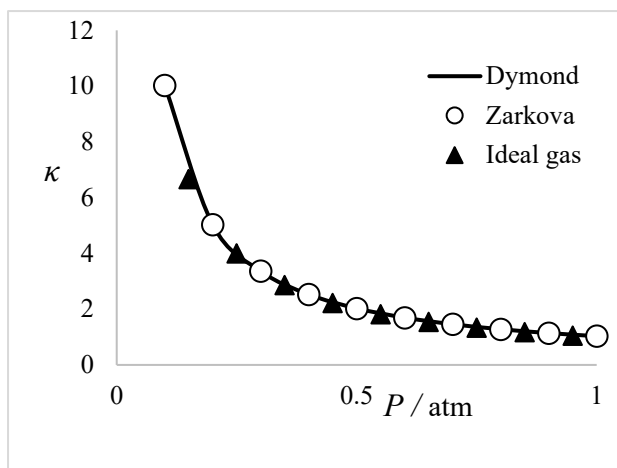


**Fig. 4.** The calculated  $A_0 = -(\partial H / \partial P)_T^0$  of  $UF_6$  versus temperature



**Fig. 7.** Variations of thermal expansion coefficient of  $UF_6$  as a function of temperature in comparison with ideal gas





**Fig. 8.** The behavior of the isothermal compressibility of  $UF_6$  vs pressure in comparison with ideal gas

## V. CONCLUSION

In this paper, we calculated and modeled some thermodynamic functions at low pressure for  $UF_6$  fluid in order to evaluate the performance of its correlation equation of second virial coefficient and virial equation of state at low pressure. A review of the figures and results shows that

1. The correlation equations presented have a good ability to predict and model the thermophysical properties of uranium hexafluoride and its deviation from the ideal state especially in the temperature range  $360 \leq T (K) \leq 500$ .
2. If the virial coefficients are accurately determined, the thermodynamic properties of fluids can be calculated and predicted with good accuracy.
3. Since virial coefficients are a connection bridge between microscopic and macroscopic properties of materials, therefore thermodynamic behavior and the non-ideal behavior of real fluids can be explained very well.
4. This approach means using accurate virial coefficients and virial equation of state (VEOS) is the suitable method for modeling many thermophysical properties of fluids.

Of course, for a more accurate judgment, other thermodynamic functions that can be calculated using the virial coefficients must be obtained. In this regard, the study of entropy deviation function, determination of intermolecular potentials via inversion method, determination of Joule-

Thomson coefficient in a wide range of temperature and pressure will be of importance. The aforementioned studies will be our future research.

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