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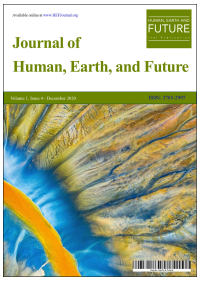

Determination of Second Virial Coefficient of Gold by a Modified Berthelot Equation of State

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Abstract

The present study aims to determine the second virial coefficient of gold over a wide range of temperatures from the boiling point to the critical point. A three - parameter modified Berthelot equation of state has been employed to determine the second virial coefficient of gold. The parameters of the equation of state are determined through the critical - point parameters of gold. The temperature -dependence of the second virial coefficient of gold has been investigated. The obtained results are compared with that of the van der Waals equation of state, Berthelot equation of state, Tsonopoulus correlation, and McGlashan correlation. The results of this work agree well with that of other correlations in the vicinity of the critical point. It is also established that gold obeys the single - parameter law of corresponding states. And, the new parameter introduced in the attractive term of the equation of state is found to be a thermodynamic similarity parameter.

*Keywords:*Equation of State; Law of Corresponding States; Gold; Second Virial Coefficient.

1. Introduction

Owing to its unique physical properties, gold has numerous scientific and technological applications in electronics, catalysis, biotechnology, spectroscopy, etc. The gold nanoparticles have applications in material science, nano-medicine, electronics, and photonics [1–15]. This fact has led to numerous experimental and theoretical studies on the thermodynamic properties of gold. The thermodynamic properties of substances are determined by the intermolecular interactions. The second virial coefficient is a measure of pairwise intermolecular interaction in substances. Thus, knowledge of the second virial coefficient will enable one to study the intermolecular interaction. Certain technological applications of gold require knowledge of their high-temperature properties [16–19]. However, the accuracy of the experimental studies on the high temperature properties of gold is poor due to severe experimental difficulties. This fact necessitates theoretical studies on the high-temperature properties of gold. Based on a three – parameter, this work deals with the determination of the second virial coefficient of gold in a wide range of temperatures, from the boiling point to the critical point [20–27].

The present research methodology has been presented in Figure 1:

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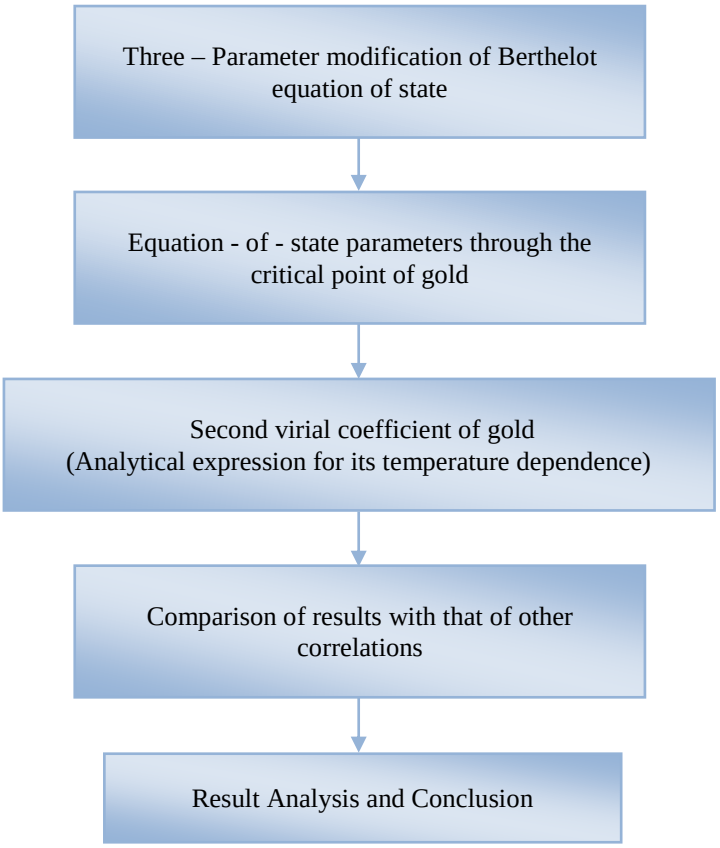

Figure 1. Flowchart of the research methodology

2. Generalized Berthelot Equation of State

The known two - parameter Berthelot equation of state does not quantitatively describe the thermodynamic properties of liquids and gases [28, 29]. Hence, in this work, an improvement to this equation is proposed by introducing a third parameter *m* in the attractive term. Such a generalized Berthelot equation of state for one mole of substance has the form:

$$P = \frac{RT}{V-b} - \frac{a}{T^m V^2} \tag{1}$$

The parameters *a*, *b* and *m* in Equation 1 may be determined through the critical - point parameters. Application of the critical-point conditions to the equation of state given by Equation 1 gives the expressions for the equation - of - state parameters as;

$$a = \frac{27RbT_c^{m+1}}{8} \tag{2}$$

$$b = \frac{V_c}{3} \tag{3}$$

$$m = \frac{\alpha_R - 4}{3} \tag{4}$$

where, T_c - critical temperature, V_c- critical volume, α_R - Riedel's parameter.

Equation 1 may be rewritten in the reduced form as;

$$P^* = \frac{8T^*}{3V^* - 1} - \frac{3}{T^{*m}V^{*2}} \tag{5}$$

where, $P^* = P/P_c$, $V^* = V/V_c$, $T^* = T/T_c$.

The reduced equation of state given by Equation 5 represents the single-parameter law of corresponding states with the thermodynamic similarity parameter *m*. That is, substances obeying the generalized Berthelot equation of state,

with the same value of parameter *m* are thermodynamically similar.

3. Determination of the Equation of-State-Parameters

Using Equations 2 to 4, the parameters *a*,*b* and *m* of the generalized Berthelot equation of state are determined through experimental data [30] on the vapor – liquid critical parameters for gold. The obtained values of the parameters *a*, *b* and *m* are presented in Table 1.

Table 1. Equation - of - state parameters for gold

a $10^{-13}Jk^{m}m^{3}/mol^{-2}$	***b*** $10^{-5}\ m^{3}/mol^{-1}$	***m***
4.260	0.852	0.874

4. Second Virial Coefficient by Generalized Berthelot Equation of State

The compressibility factor may be expressed in terms of a series in $1/V$ to get the virial equation of state as [31];

$$Z \equiv \frac{PV}{RT} = 1 + \frac{B_2}{V} + \frac{B_3}{V^2} + ... \tag{6}$$

Where, B_2 - second virial coefficient, B_3 - third virial coefficient and so on.

For a given substance, the virial coefficient depend only on temperature. In fact, the second virial coefficient is a measure of pair-wise intermolecular interaction. And, the third virial coefficient is a measure of intermolecular interaction between three molecules. Hence, the knowledge of the virial coefficient will enable one to determine the intermolecular potential of substances. In general, reliable data on the virial coefficient of substances are scarce.

The second virial coefficient of substances are determined from the equilibrium *PVT* properties.The second virial coefficient is given by [32];

$$B_2 = \left(\frac{\partial Z}{\partial \rho}\right)_T \text{ at } \rho = 0 \tag{7}$$

where, $\rho$is the molar density.

For fluids obeying Equation 1, the compressibility factor is;

$$Z = \frac{1}{1-b\rho} - \frac{a\rho}{RT^{m+1}} \tag{8}$$

From Equations 7 and 8, we get the second virial coefficient of fluids obeying Equation 1 as;

$$B_2 = b - \frac{a}{RT^{m+1}} \tag{9}$$

The second virial coefficient may be reduced through the critical volume as;

$$B_2^* = \frac{B_2}{V_c} \tag{10}$$

Hence, we get;

$$B_2^* = \frac{1}{3} - \frac{9}{8T^{*m+1}} \tag{11}$$

5. Second virial Coefficient of gold

The second virial coefficient of gold at various temperatures are determined by Equation 11 with the value the parameter *m* presented in Table 1. The obtained values of the second virial coefficient for gold are presented in Table 2. For comparison, the second virial coefficient of gold is also determined through the Tsonopoulus correlation [33], McGlashan correlation [34], van der Waals and Berthelot equations of state. The results are also presented in Table 2. The temperature dependence of the second virial coefficient of gold is also plotted in Figure 2.

Table 2. Second virial coefficient of gold

T*	B_2*				
	Eq.(11)	McGlashan correlation [34]	Berthelot EoS	Tsonopoulos correlation[33]	van der Waals EoS
0.60	-1.726	-2.359	-2.792	-2.903	-1.542
0.62	-1.647	-2.214	-2.593	-2.691	-1.481
0.64	-1.574	-2.082	-2.413	-2.501	-1.424
0.66	-1.506	-1.962	-2.249	-2.332	-1.371
0.68	-1.442	-1.853	-2.099	-2.179	-1.321
0.70	-1.382	-1.753	-1.963	-2.041	-1.274
0.72	-1.326	-1.662	-1.837	-1.916	-1.229
0.74	-1.273	-1.578	-1.721	-1.802	-1.187
0.76	-1.223	-1.450	-1.614	-1.698	-1.147
0.78	-1.176	-1.428	-1.516	-1.603	-1.109
0.80	-1.132	-1.361	-1.424	-1.515	-1.073
0.82	-1.089	-1.299	-1.340	-1.434	-1.039
0.84	-1.019	-1.240	-1.261	-1.359	-1.006
0.86	-1.011	-1.186	-1.188	-1.289	-0.975
0.88	-0.975	-1.135	-1.119	-1.225	-0.945
0.90	-0.941	-1.087	-1.055	-1.164	-0.917
0.92	-0.908	-1.043	-0.996	-1.108	-0.889
0.94	-0.877	-1.000	-0.939	-1.055	-0.863
0.96	-0.847	-0.960	-0.887	-1.006	-0.839
0.98	-0.819	-0.923	-0.838	-0.960	-0.815
1.0	-0.792	-0.887	-0.791	-0.916	-0.792

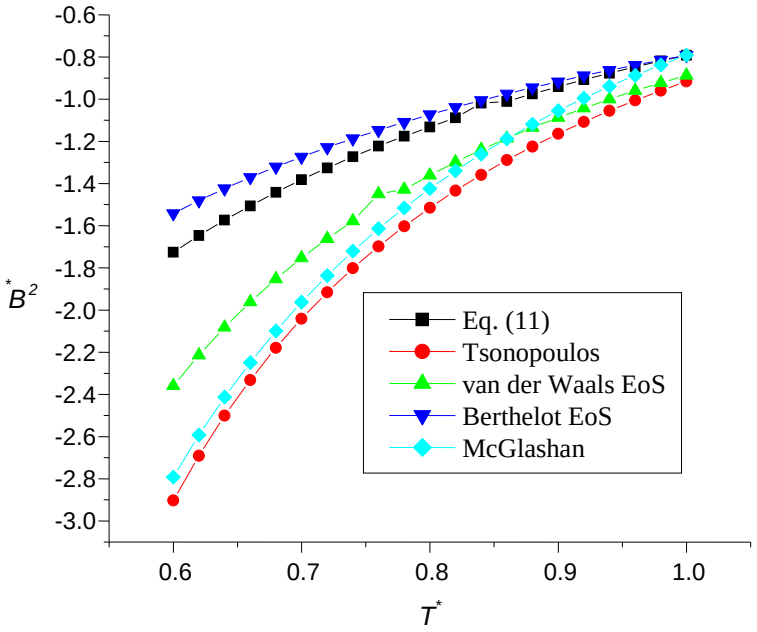

Figure 2. Second virial coefficient of gold

The generalized Bertholet equation of state has been employed to calculate the second virial coefficient of gold. As seen from Table 2, the generalized Berthelot Equation of State gives higher values of the second virial coefficient compared to the Tsonopoulus correlation, the McGlashan correlation, and the Berthelot equation of state. But, the generalized Berthelot Equation of State gives a smaller value of the second virial coefficient compared to the van der Waals equation of state. In the vicinity of the critical point, this discrepancy greatly decreases.

6. Conclusion

The second virial coefficient in a wide range of temperatures from the boiling point to the critical point of gold has been determined using the generalized Berthelot equation of state. A single - parameter law of corresponding states based on the generalized Berthelot equation of state has been derived. It is established that the introduced parameter m is a thermodynamic similarity parameter of substances. The obtained results agree with those of other correlations in the high temperature region, i.e., in the vicinity of the critical point.

7. Declarations

7.1. Author Contributions

Conceptualization, R.B.; methodology, R.B.; software, M.S.; validation, M.S.; formal analysis, R.B.; investigation, M.S.; data curation, M.S.; writing—original draft preparation, R.B.; writing—review and editing, R.B. All authors have read and agreed to the published version of the manuscript.

7.2. Data Availability Statement

The data presented in this study are available in article.

7.3. Funding

The authors received no financial support for the research, authorship, and/or publication of this article.

7.4. Institutional Review Board Statement

Not applicable.

7.5. Informed Consent Statement

Not applicable.

7.6. Declaration of Competing Interest

The authors declare that there is no conflict of interests regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies have been completely observed by the authors.

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