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An intensified analytic solution for finding the roots of a cubic equation of state in low temperature region

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ABSTRACT

Because of the effect of the enlarging process of errors in low temperature region, the analytical solutions of a cubic equation of state (CES) lead to illogical results. To overcome this problem, we recommend an enhanced analytic method, in this paper. Up to now, there is not any analytical method for this problem. In the present study, the general cubic equation $x^3 + Bx^2 + Cx + D = 0$ is transformed into simple equation $\gamma^3 - \beta\gamma + \beta = 0$. For $\beta \geq 27/4$, then the three roots are real. To compare, as an example, for 1-butene at $T = 112.3$ (K) and $P = 3.79 \times 10^{-9}$(Pa), the empirical value of the molar volume is 72.00 ($\text{m}^3\text{mol}^{-1}$). By using Patel–Teja (PT) CES, the molar volume value is obtained as −342.3 from traditional analytic method and 73.88 from both the new intensified analytic method and the iterative Newton–Raphson method.

1. Introduction

The CES models are useful formulas for analyzing and correlating the thermodynamic equilibrium state of simple fluids and their mixtures, with agreeable approach [1–5]. Generally, for a given substance, the CES is an empirical relation of the pressure P, the temperature T and the molar volume v consist of a repulsive term and an attractive term as follows [6]:

$$P(T,v) = \frac{RT}{v-b} - \frac{\alpha(T)}{(v-c)(v-d)} \tag{1}$$

where R is the gas constant. b, c and d are constant parameters which are obtained based on the kind of equation. In Eq. (1), $\alpha(T)$ is a function and it has many empirical definitions in the literature. By expressing Eq. (1) in terms of molar volume, the following equation is obtained:

$$v^3 - \left(b + c + d + \frac{RT}{P}\right)v^2 + \left(bc + bd + cd + \frac{RT}{P}c + \frac{RT}{P}d + \frac{\alpha(T)}{P}\right)v - \left(bcd + \frac{RT}{P}cd + \frac{\alpha(t)}{P}b\right) = 0. \tag{2}$$

Eq. (2) is referred to as cubic in molar volume. Additionally we can substitute the definition of compressibility factor (i.e., $Z = Pv/RT$) into Eq. (2) and obtain different cubic equations in Z.

The first CES was recommended by van der Waals in 1873 as $P(T,v) = RT/(v-b) - \alpha(T)/v^2$. It has been proven that the original van der Waals CES cannot provide simultaneous accurate predictions for all the properties of pure fluids and their mixtures. But, the most CES models (e.g., Peng-Robison CES in 1976 as $P(T,v) = RT/(v-b) - \alpha(T)/(v^2 + 2bv - b^2)$ being used widely today for practical design purposes have been derived from van der Waals CES [7].

For finding the roots of Eq. (2), the analytical methods can solve their three roots simultaneously. One of the relevant math formulas is the well-known formula due to Ferro and Tartaglia, communicated by Gerolamo Cardano in 1545 [8,9].

Cardano's method involves division. Thus it can encounter near "0/0", resulting insignificant numerical errors. Thus it may encounter a numerically unstable case. Lagrange in 1770 gave the new method for solving the three roots of a cubic equation, with 18 possible interpretations [10]. The Lagrange formula, does not require division and thus avoids the "0/0" case. In the Lagrange formula some interpretations are correct (yielding the solutions), But the others are not. Zhao et al. [11] proposed a convection which provided correct interpretations of the Lagrange formula for all cubic equations with real coefficients.

Zhi and Lee [12] revealed by several examples that, in low temperature region, the analytical solutions of CES lead to irrational results, while the iterative solutions of the CES, using Newton–Raphson method produced valid results. They appeared that errors caused by the limitation of significant figures of the computer languages are revealed, and a magnification of errors is defined which a main factor is bringing out the irrational results of the analytical solution of CES. Salim [13] showed that, in the case of low temperature region, the coefficient D in cubic equation $x^3 + Bx^2 + Cx + D = 0$ is very small. Therefore the main root is also small and becomes so close to zero. Thus, by eliminating the term of x^3 in $x^3 + Bx^2 + Cx + D = 0$, then the main root can be

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found via the approximated equation of the form $Bx^2 + Cx + D = 0$. Loperena [14] proposed an iterative refinement of the solution obtained by the analytical method. This method allowed one to take advantage of the calculations fulfilled in the application of the analytical solution. His numerical results show that the proposed iterative refinement procedure is an attractive and numerical inexpensive option and can be easily incorporated into any process simulation program, that use Cardano's method, without significant modifications.

Up to now, as mentioned above discussions, there is not any completely analytical method for this problem. To notice to complexity and overhead of analytical methods, it has been recommended to use the numeric iterative methods. In this paper, we describe an enhanced completely analytic method for solving the general cubic equation $x^3 + Bx^2 + Cx + D = 0$ consists of real coefficients. We verify this new method with the miscellaneous examples.

2. New analytic solution and the miscellaneous examples

An arbitrary cubic equation which consists of real coefficients B, C and D is as follows:

$$x^3 + Bx^2 + Cx + D = 0. \tag{3}$$

In Eq. (3), one of the three roots is real. To find it, let $\beta = -\frac{C_1^3}{D_1^2}$, where $C_1 = 9C - 3B^2$ and $D_1 = 2B^3 - 9BC + 27D$. Make the substitution $x = -\frac{1}{3}\left(\sqrt[3]{(1-\gamma)D_1} + B\right)$ or $x = -\frac{1}{3}\left(\frac{D_1}{C_1}\gamma + B\right)$. By this substitution, Eq. (3) is transformed as the following simple equation for γ:

$$\gamma^3 - \beta\gamma + \beta = 0. \tag{4}$$

To find γ, we arrange Eq. (4) into the functional form as $\beta(\gamma) = \frac{\gamma^3}{\gamma - 1}$. Fig. 1 shows the sketch of $\beta(\gamma)$. It is seen that for $\beta \geq \frac{27}{4}$, then all three roots are real. Therefore, Eq. (3) has three real roots (i.e., x_1, x_2, x_3). Also, for $\beta < \frac{27}{4}$, Eq. (3) has one real root (i.e., x_1). In this case, the others are conjugate imaginary roots (i.e., x_2, x_3).

Therefore, like a new analytic method, for finding the one real root of a cubic equation, let $x_1 = -\frac{1}{3}\left(\sqrt[3]{(1-\gamma)D_1} + B\right)$ or $x_1 = -\frac{1}{3}\left(\frac{D_1}{C_1}\gamma + B\right)$ be one real root of Eq. (3), where γ is related with the left branch of the curves β in Fig. 1 (i.e., $\gamma \leq 1$); and it is obtained from the following formula as:

$$\begin{cases} \gamma = \left(-\dfrac{\beta}{2} + \sqrt{\dfrac{\beta^2}{4} - \dfrac{\beta^3}{27}}\right)^{\frac{1}{3}} + \left(-\dfrac{\beta}{2} - \sqrt{\dfrac{\beta^2}{4} - \dfrac{\beta^3}{27}}\right)^{\frac{1}{3}}, & \text{for } \beta \leq \dfrac{27}{4} \\ \gamma = -2\sqrt{\dfrac{\beta}{3}}\cos\theta, \quad \theta = \dfrac{1}{3}\cos^{-1}\left(\dfrac{9}{\sqrt{12\beta}}\right), & \text{for } \beta \geq \dfrac{27}{4}. \end{cases} \tag{5}$$

It is clear that (see Fig. 1), when $\beta \to -\infty$, then $\gamma \to 1$. Also, when $\beta \to +\infty$, then $\gamma \to -\infty$.

To obtain the two formulas in Eq. (5), an analytic method was completely used. This method has been described in Appendix A. Therefore, through an intensified analytic solution, the real root of the cubic Eq. (3) is captured.

The other roots of Eq. (3) i.e., x_2, x_3 can be calculated analytically from the following quadratic equation as:

$$x^2 + (B + x_1)x - \frac{D}{x_1} = 0. \tag{6}$$

Note that, in order to reach the high precision of the solutions, especially in low temperature region, the two other roots may be obtained from Eq. (6). In this paper, all solutions were conducted by Microsoft Excel, 2003.

Example 1. In equation: $x^3 - 3x^2 + 4x - 2 = 0$, the coefficients are: $B = -3$, $C = 4$ and $D = -2$. Then, $C_1 = 9$ and $D_1 = 0$. Therefore, $\beta = -\infty$. Thus, from Fig. 1: $\gamma = 1$. Therefore, $x_1 = -B/3 = 1$. Finally from Eq. (6): $x^2 - 2x + 2 = 0$. Then, $x_2 = 1 + i$ and $x_3 = 1 - i$.

Example 2. In equation: $x^3 + 6x^2 + 3x - 10 = 0$, the coefficients are: $B = 6$, $C = 3$, $D = -10$. Then $C_1 = -81$ and $D_1 = 0$. Therefore, $\beta = +\infty$. Thus, from Fig. 1: $\gamma = -\infty$. Therefore, $x_1 = -B/3 = -2$. Finally from Eq. (6): $x^2 + 4x - 5 = 0$. Then, $x_2 = 1$ and $x_3 = -5$.

Example 3. In equation: $x^3 - 2x^2 - 5x + 6 = 0$, the coefficients are: $B = -2$, $C = -5$, $D = 6$. Then $C_1 = -57$ and $D_1 = 56$. Then, $\beta = 59.0539$. Thus, from Eq. (5): $\gamma = -8.1429$. Therefore, $x_1 = -2.0000$. Finally from Eq. (6): $x^2 - 4x + 3 = 0$. Then, $x_2 = 1.0000$ and $x_3 = 3.0000$.

Example 4. The cubic equation: $(x-1)^2 x = x^3 - 2x^2 + x = 0$. The coefficients are: $B = -2$, $C = 1$, $D = 0$. Then $C_1 = -3$ and $D_1 = 2$. Then, $\beta = 6.75$. Thus, from Eq. (5): $\gamma = -3$. Therefore, $x_1 = 0$. Finally from solution of the equation: $x^2 - 2x + 1 = 0$, we have: $x_2 = x_3 = 1.0000$.

Example 5. The molar volume of carbon dioxide (CO_2) at $P = 10$ atm and $T = 300$ K, by using the van der Waals CES ($P(T, v) = RT/(v - b) - \alpha(T)/v^2$), is the cubic equation as: $v^3 - 2.5046v^2 + 0.3598v - 0.0155 = 0$. This equation and another equation in the form of $v^3 - 7.8693v^2 + 13.3771v - 6.5354 = 0$

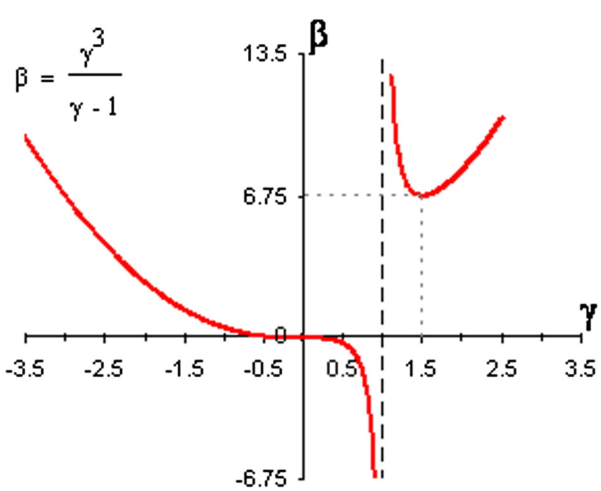

Fig. 1. The curve of $\beta(\gamma)$.

Table 1
Results for example 5.

	Case I: $v^3 - 2.5046v^2 + 0.3598v - 0.0155 = 0$	Case II: $v^3 - 7.8693v^2 + 13.3771v - 6.5354 = 0$
Newton (numeric)	*Iterations*→ 2.4616, 2.3633, 2.3546, 2.3545→v_1	*Iterations*→ 7.3807, 6.2992, 5.8355, 5.7397, 5.7357→v_1
Ostrowski [15] (numeric)	*Iterations*→ 2.4616, 2.3545→v_1	*Iterations*→ 7.3807, 5.8187, 5.7357→v_1
New (analytic)	$\beta = 6.7165$, $\gamma = -2.9934$, $v_1 = 2.3545$	$\beta = 6.7396$, $\gamma = -2.9977$, $v_1 = 5.7357$