

Volume Estimation of Sour Natural Gas Using Volume Translation Peng-Robinson with Translation Equation as a Function of Molecular Weight and Acentric Factor

Desi Budi Ariani*, Mahmud Sudibandriyo*

Department of Chemical Engineering, Faculty of Engineering, University of Indonesia, Depok, Indonesia

Abstract

Research and development to improve sour natural gas volume estimation accuracy are continuously done to upgrade the industrial sectors. The accurate volume of sour natural gas is necessary for engineering calculation. The most accurate way to obtain the real volume is by performing experiments. However, it is expensive and time-consuming to obtain sour natural gas volume with a wide variety of compositions and conditions. The volume estimation accuracy can be achieved by applying chemistry and mathematics. Natural gas volume in a specific composition, temperature, and pressure can be estimated by equation of state. Peng-Robinson (PR) equation of state, usually used in the natural gas industry, has some drawbacks in calculating volume accurately. In this paper, Volume Translation Peng-Robinson (VTPR) is applied by adding the translation equation to modified PR in $T_r=0.8-1.08$ and $P=12.38-30.38$ MPa based on well P. To simplify the volume estimation for various compounds, translation equations parameters will depend on compound characteristic. Previous researches had formulated translation equations as the function of two compound characteristics which are molecular weight and acentric factor. However, H_2S and CO_2 have not been involved yet. In this study, three VTPR will be formulated with translation equation as the function of molecular weight, acentric factor, and both to estimate the volume of sour natural gas accurately. Parameters are optimized using regression to get the translation equation so that the calculated volume can approach the real volume. The result is that three VTPR have lower Average Absolute Deviation percentage (%AAD) than PR to estimate pure compound volume in sour natural gas which are 2.07%, 1.05%, and 1.47% respectively. When it is applied to sour natural gas mixture, The %AAD are 0.03618%, 0.00097%, 0.00825%, respectively. It can be concluded that these VTPR could provide accurate sour natural gas volume estimation.

* Corresponding author:

uidepokdesi@gmail.com

msudibandriyo@yahoo.com

Received 11 April 2022,

Revised 23 April 2022,

Accepted 25 May 2022

Keywords: Sour natural gas; volume translation peng-robinsons; molecular weight; acentric factor

1. Introduction

According to the International Energy Agency (IEA) report in 2019, gas consumption is forecasted to exceed 4.3 trillion cubic meters in 2024^[1]. However, more than 40% of the world's gas reserves are sour containing significant levels of acidic compounds such as CO₂ and H₂S^[2]. Natural gas is usually considered as sour gas if there is more than 5.7 mg H₂S/m³ of natural gas which is equivalent to about 4 ppm volume at standard temperature and pressure^[2]. Based on H₂S concentration in natural gas, natural gas fields are categorized into 5 types which are pure sour gas field (>70%), highly concentrated sour gas field (2%-70%), low concentrated sour gas field (0.5%-2%), tracing concentrated sour gas field (<0.5%) and H₂S free gas field^[3]. The increasing demand for natural gas as well as the availability of acidic compound content in natural gas forces the gas industry to improve the performance of gas treatment. Volumetric properties in the system are very important in facing this challenge. The hydrocarbons and acidic gases in sour natural gas affect the volumetric properties while a system at a certain composition, temperature, and pressure will have a certain volume either in the liquid phase, gas phase, or mixed phase. Accurate natural gas volume is required in the calculation of reservoir engineering, mass and energy balances, simulation of process units and operating units^[4, 5]. The most accurate way to get the real volume of sour natural gas is to perform the small-scale experiment before it is applied for the industrial scale. However, it is considered uneconomical and taking a long time to obtain the volume of natural gas which has a variety of compounds and conditions^[6]. Moreover, H₂S and CO₂ in sour natural gas are corrosive and can cause damage to equipment^[7]. The equation of state can determine the volume of sour natural gas easier by correlating pressure, temperature, and volume of substances. The equation of state is used to describe the volumetric and phase behavior, vapor and liquid equilibrium, and the thermal properties of both mixed and pure substances^[8]. However, PR estimates reservoir fluid volume in the gas phase with 3-5% error and liquid phase with 6-12% error^[9]. The large deviation could not be accepted in the industry, to overcome this deficiency a volume translation method has been developed. In this study, VTPR is applied by adding a translation equation to modified PR in $Tr=0.8-1.08$ and $P=12.38-30.38$ MPa based on well P condition which has not been analyzed in previous research. To simplify the volume estimation for various compounds, VTPR is composed of general translation equations which parameters depend on each compound characteristic. Previous researches had formulated translation equations as the function of two compound characteristics which are molecular weight and acentric factor^[9-11]. However, H₂S and CO₂ have not been involved yet. In this study, three VTPR will be formulated with translation equation as the function of molecular weight, acentric factor, and both to estimate the volume of sour natural gas accurately. The purpose of this study is to compare and analyze the three VTPR accuracy in estimating the volume of pure compounds in sour natural gas and the volume of sour natural gas mixed compounds.

2. Literature Review

2.1. Peng-Robinson (PR) Equation of State

A study which had been done by Peng & Robinson proposes the equation of state is shown in equation (1). In equation (1), R is the ideal gas constant which is $8.314 \text{ cm}^3 \cdot \text{MPa} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$, T is the temperature, and P is the pressure. The first and second derivatives of pressure in equation (1) at a critical point with respect to volume can obtain expressions for a and b which are shown in equations (2) and (3). The dimensionless scaling factor (α) for the parameter a which is shown in equations (2) and (4) as a function of acentric factor and reduced temperature (Tr) has significantly improved the prediction of vapor pressures for pure substances and consequently the equilibrium ratios for mixtures^[12]. However, PR estimates reservoir fluid volume in the gas phase with 3-5% error and liquid phase with 6-12% error^[9]. In addition, the prediction of liquid density using PR is not accurate in the area near the critical point^[13, 14]. The

inaccuracy of PR in calculating the liquid density at conditions near the critical point occurs because the critical compressibility factor (Z_c) parameter for all fluids is universal^[13].

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \quad (1)$$

$$a(T) = \frac{0.45724 R^2 T_c^2}{P_c} \alpha(T) \quad (2)$$

$$b = \frac{0.0778 RT_c}{P_c} \quad (3)$$

$$\alpha(T) = \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{T_r}) \right]^2 \quad (4)$$

2.2. Volume Translation Peng-Robinson (VTPR)

The volume translation method is to shift the volume axis to increase the accuracy of the prediction of volume without causing changes in vapor and liquid equilibrium^[15]. The volume translation is done by adding correction constants or translation equations. Peneloux has developed a volume correction constant in the Soave Redlich Kwong (SRK) equation of state which can significantly improve the volume prediction of liquids at low reduced temperatures. However, the density value obtained at a reduced temperature above 0.7 and in the very high pressure has large deviations^[15].

$$v^{VTPR} = v^{PR} - c \quad (5)$$

In equation (1), the correction constant or translation equation is symbolized as c , while v^{PR} is the molar volume calculated by PR equation of state, and v^{VTPR} is the translated molar volume of PR equation of state. PR equation of state is shown in equation (1). The translation equation requires several additional parameters obtained from experimental data for each compound. This of course requires high costs and takes a long time. To overcome this difficulty, the general equation is needed where the parameter depends on the compound characteristics. Previous research has formulated equations where parameters are a function of molecular weight, acentric factors, and both for various pure compounds. However, volume estimation of natural gas mixtures using translation equations as a function of molecular weight, acentric factors, and both in which reference data involve H_2S and CO_2 has not been done yet.

3. Methodology

The structured steps are described in a flow chart which is shown in Fig. 1. Three VTPR equations which consist of the translation equation as a function of molecular weight, the translation equation as a function of the acentric factor, and the translation equation as a function of molecular weight and acentric factor will be formulated. The formulation of the translation equation was carried out using Microsoft Excel and MATLAB software by using a curve-fitting tool. The value of c obtained from the difference between the volume of NIST reference data and the volume obtained from the PR equation of state is regressed to get the parameters (k) in VTPR equations. The volume obtained from the VTPR will be sought to calculate %AAD from the reference data. Because PR equation estimates reservoir fluid volume with 3-12% error^[9], The %AAD limitation is determined to be 2.5% to make a better volume estimation. Before calculating the volume of the sour natural gas mixture, the %AAD of the pure components needs to be limited to 2.5% to ensure that the translation equation can be used to estimate the volume of pure compounds in the sour natural gas accurately. The VTPR is formulated for all pure compounds at $Tr=0.8-1.08$ and $P=12.38-30.38$ MPa. The sour natural gas composition and condition which are analyzed in this study are based on well P in Indonesia. The composition of the analyzed sour natural gas is shown in Table 1.

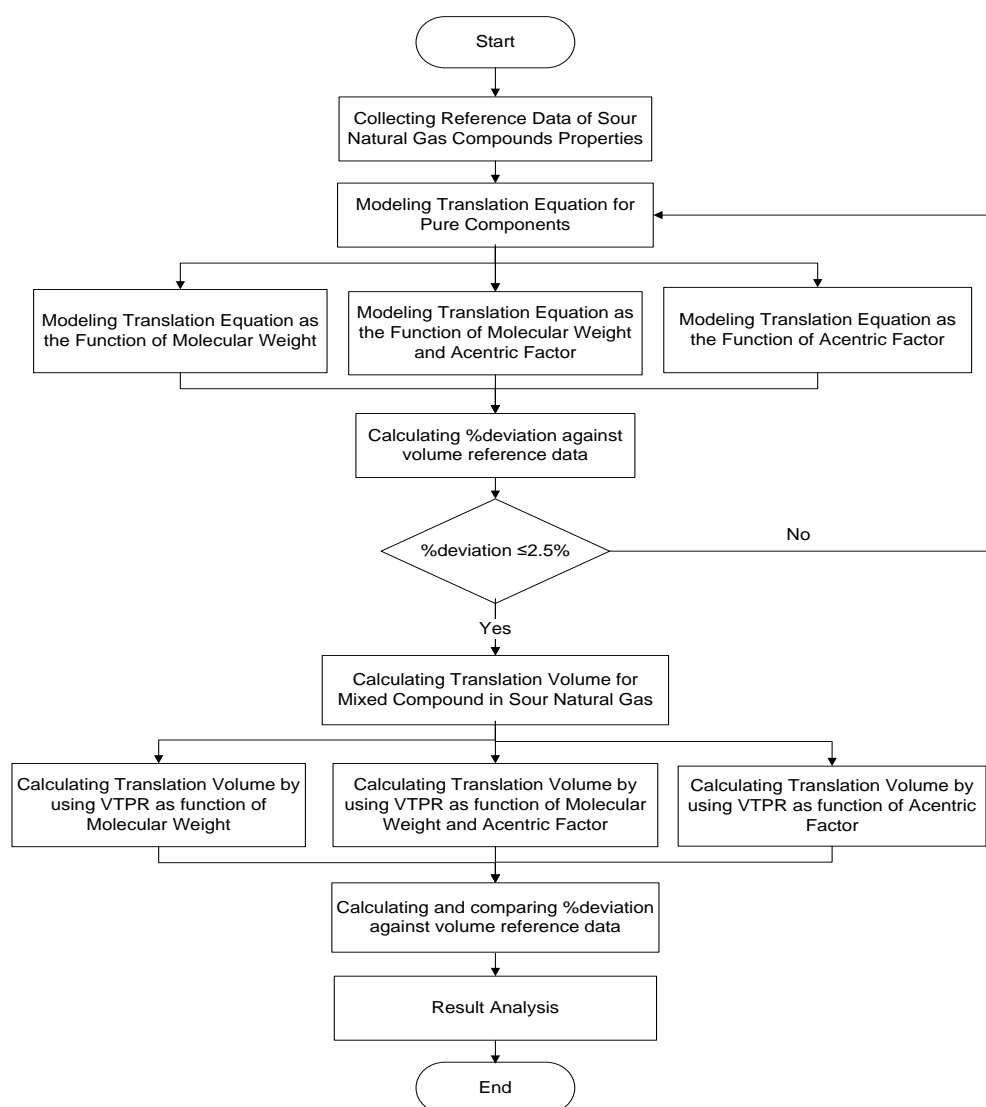


Figure 1: Research Method Flow Chart

Table 1: Composition of Analyzed Sour Natural Gas

Compounds	Mole Fraction	Compounds	Mole Fraction	Compounds	Mole Fraction
N ₂	0.0065	C ₂	0.1027	iC ₅	0.0050
CO ₂	0.0001	C ₃	0.0532	C ₅	0.0030
H ₂ S	0.0038	iC ₄	0.0141	C ₆	0.0048
C ₁	0.7720	C ₄	0.0119	C ₇	0.0229

4. Results Analysis

4.1. VTPR as a Function of Molecular Weight

Nonlinear regression is applied to determine the parameters of the translation equation shown in Equation (6) in which c is the translation value, b is the second parameter of the PR equation, M is the molecular weight, k_1 and k_2 are the translation parameters whose values need to be optimized. Previous research formulated this translation equation involving molecular weight which resulted in deviations of less than 0.3% for hydrocarbon heavier than heptane at conditions $T = 60^\circ\text{F}$ and 1 atm to characterize the pseudo component of the hydrocarbon fraction^[9]. However, that study has not analyzed H₂S and CO₂ compounds. In this paper, VTPR equation depends on the reduced temperature

with the equation parameters correlated with the molecular weight. Several VTPR equations use polynomials or powers involving reduced temperatures to provide flexibility of use for a wider range of temperatures^[16]. Parameters are correlated to the reduced temperature and the molecular weight of the analyzed compounds in sour natural gas which is shown in Table 2.

$$\frac{c}{b} = 1 - \frac{k_1}{M^{k_2}} \quad (6)$$

$$k_1 = k_3 Tr^2 + k_4 Tr + k_5 \quad (7)$$

$$k_2 = k_6 Tr^2 + k_7 Tr + k_8 \quad (8)$$

CO₂ when applying the equation (6)-(8), produces %AAD which is higher than %AAD of the PR equation. The molecular weight involvement gives a high relative error in the regression. This might happen because the formulation is not suitable enough to represent the volume of analyzed compounds in the area near critical temperature, especially with H₂S and CO₂. Therefore, for the compound which has %AAD higher than the PR equation, equation (9) is used to obtain %AAD lower than 2.5%.

$$\frac{c}{b} = \frac{\left(1 - \frac{k_1}{M^{k_2}}\right)}{M} \quad (9)$$

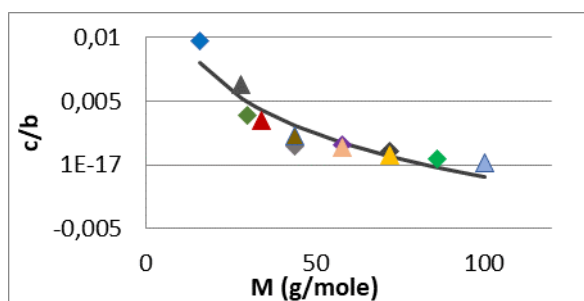
Table 2: Translation Equation Parameters as a Function of Molecular Weight

Pressure (MPa)	k ₃	k ₄	k ₅	k ₆	k ₇	k ₈
12.38	1.85 × 10 ⁻¹	-2.87 × 10 ⁻¹	1.09	3.11 × 10 ⁻²	-4.52 × 10 ⁻²	1.13 × 10 ⁻²
14.38	1.37 × 10 ⁻¹	-2.07 × 10 ⁻¹	1.06	3.38 × 10 ⁻²	-5.28 × 10 ⁻²	1.56 × 10 ⁻²
16.38	1.16 × 10 ⁻¹	-1.82 × 10 ⁻¹	1.05	2.97 × 10 ⁻²	-4.70 × 10 ⁻²	1.37 × 10 ⁻²
18.38	5.33 × 10 ⁻²	-6.97 × 10 ⁻²	0.99	2.32 × 10 ⁻²	-3.64 × 10 ⁻²	9.30 × 10 ⁻³
20.38	9.11 × 10 ⁻²	-1.45 × 10 ⁻¹	1.04	1.94 × 10 ⁻²	-3.06 × 10 ⁻²	7.10 × 10 ⁻³
22.38	6.80 × 10 ⁻²	-1.04 × 10 ⁻¹	1.02	1.62 × 10 ⁻²	-2.56 × 10 ⁻²	5.10 × 10 ⁻³
24.38	6.80 × 10 ⁻²	-1.10 × 10 ⁻¹	1.02	1.38 × 10 ⁻²	-2.19 × 10 ⁻²	3.70 × 10 ⁻³
26.38	5.68 × 10 ⁻²	-9.22 × 10 ⁻²	1.02	1.19 × 10 ⁻²	-1.91 × 10 ⁻²	2.60 × 10 ⁻³
28.38	1.15 × 10 ⁻¹	-1.99 × 10 ⁻¹	1.06	1.05 × 10 ⁻²	-1.69 × 10 ⁻²	1.80 × 10 ⁻³
30.38	4.72 × 10 ⁻²	-7.90 × 10 ⁻²	1.01	9.30 × 10 ⁻³	-1.51 × 10 ⁻²	1.10 × 10 ⁻³

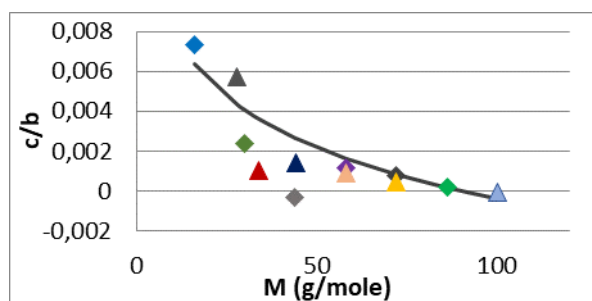
The %AAD of this VTPR equation when it is applied to the analyzed pure compound is 2.07%. VTPR with this parameter as a function of molecular weight has a lower deviation value than the PR equation but higher than the other two VTPR equations shown in Table 3. Research conducted by previous research concluded that the application of the VTPR using equation (6) results in a poor volumetric estimate for the pure component around the critical point^[9]. It was justified that the needed correction for volume estimation is nearly constant up to a reduced temperature of 0.75 and then it changes rapidly when it is near the critical region^[11]. The CO₂ and H₂S compounds gave a high relative error in regression which is shown in Fig. 2. Compared to other analyzed hydrocarbon compounds, H₂S and CO₂ have critical pressure (P_c) close to the pressure analyzed in this study which is 7.3773 MPa and 9 MPa for CO₂ and H₂S respectively. Pure compounds in sour natural gas at a pressure of 12.38 MPa and a reduced temperature of 0.8-0.89 have a small relative error in the translation equation modeling. However, as the reduced temperature increases, the relative error increases especially H₂S and CO₂. The regression of the volume translation equation applied to pressures above 12.38 MPa resulted in a smaller relative error. Meanwhile, for each pressure analyzed, which is 12.38 - 30.38 MPa, the relative error will be higher with increasing reduced temperature the same as the phenomena that occur at a pressure of 12.38 MPa as shown in Fig. 2.

Table 3: The comparison of VTPR and PR Deviation

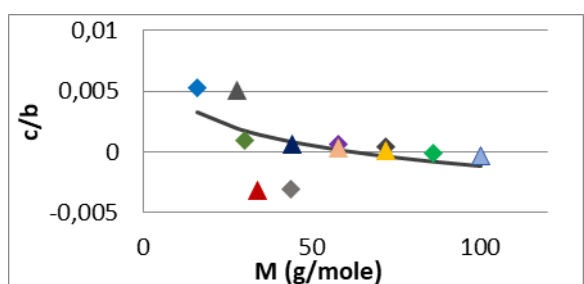
Compounds	M (g/mole)	ω	$-1/(M\omega)$	%AAD PR	%AAD VTPR $c = f(M)$	%AAD VTPR $c=f(M,\omega)$	%AAD VTPR $c = f(\omega)$
C1	16.043	0.0114	-5.4582	8.4437%	1.6606%	0.3132%	0.8845%
C2	30.069	0.0995	-0.3342	6.2491%	1.8756%	0.9907%	0.5800%
C3	44.096	0.1521	-0.1490	5.7886%	2.0180%	0.6954%	0.3518%
iC4	58.122	0.1840	-0.0935	5.9107%	1.2900%	1.2920%	0.9889%
C4	58.122	0.2010	-0.0856	5.1014%	1.5347%	1.0631%	0.5585%
iC5	72.149	0.2274	-0.0609	5.3954%	2.2273%	1.5900%	1.4640%
C5	72.149	0.2510	-0.0552	3.9039%	1.4525%	1.2264%	0.4859%
C6	86.175	0.2990	-0.0388	2.9632%	2.7022%	1.3260%	0.5511%
C7	100.2	0.3490	-0.0286	1.6953%	1.6536%	1.4904%	0.4678%
N ₂	28.013	0.0372	-0.9596	10.5162%	2.4418%	3.1920%	2.5254%
CO ₂	44.010	0.2239	-0.1014	3.1933%	3.1089%	2.3159%	1.9119%
H ₂ S	34.081	0.1005	-0.2919	4.7952%	2.8745%	2.1076%	1.7975%
%AAD Total				5.3297%	2.0700%	1.4669%	1.0473%



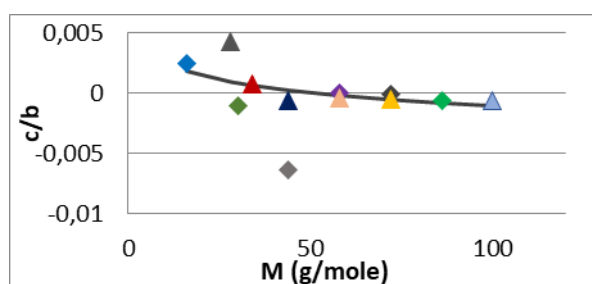
(a)



(b)



(c)

(c) C1 ▲ N₂ ◆ C2 ▲ H₂S ◆ CO₂ ▲ C3 ◆ iC4 ▲ C4 ◆ iC5 ▲ C5 ◆ C6 ▲ C7 — Regression**Figure 2:** Parameter Optimization of VTPR as a Function of Molecular Weight of Each Pure Compound in Sour Natural Gas (a) P = 12.38 MPa, Tr = 0.8 (b) P = 12.38 MPa, Tr = 0.95 (c) P = 12.38 MPa, Tr = 1.02 (d) P = 12.38 MPa, Tr = 1.08

4.2. VTPR as a Function of Molecular Weight and Acentric Factor

The modeling of the VTPR equation as a function of the acentric factor and molecular weight, carried out by previous studies, did not involve CO₂ and H₂S compounds in determining the parameters of the translation equation^[10]. This research will use the VTPR equation shown in equations (10) and (11) involving CO₂ and H₂S compounds. Linear

regression is applied in which c is the volume translation value which is a function of the reduced temperature. Parameters C_1 and C_2 are obtained from parameter optimization at the reduced temperature of 0.8-1.08 for each compound in sour natural gas. Parameters C_1 and C_2 are correlated with the specific properties of the compound which are the molecular weight (M) and acentric factor (ω) as shown in equation (11).

$$c = C_1 + C_2 \cdot T_r \quad (10)$$

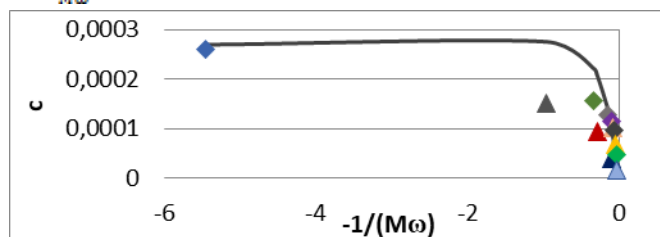
$$C_1, C_2 = f(M, \omega) = k_0 + k_1 \exp\left(\frac{-1}{k_2 M \omega}\right) + k_3 \exp\left(\frac{-1}{k_3 M \omega}\right) + k_4 \exp\left(\frac{-1}{k_4 M \omega}\right) \quad (11)$$

Table 4: Translation Equation Parameters as a Function of Molecular Weight and Acentric Factor

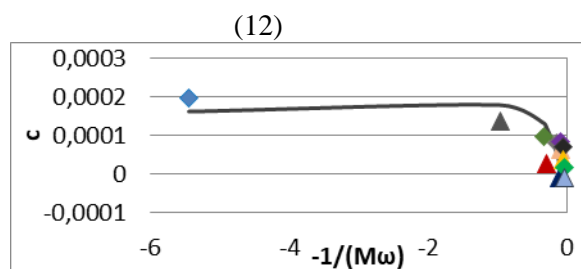
P (MPa)	C ₁					C ₂				
	k ₀	k ₁	k ₂	k ₃	k ₄	k ₀	k ₁	k ₂	k ₃	k ₄
12,38	-7.02 × 10 ⁻⁴	1.37 × 10 ⁻⁴	0.158	1.560	0.039	8.29 × 10 ⁻⁴	-1.90 × 10 ⁻⁴	0.7307	0.1253	0.1369
14,38	-5.36 × 10 ⁻⁴	8.49 × 10 ⁻⁵	0.234	0.702	0.250	7.06 × 10 ⁻⁴	-1.60 × 10 ⁻⁴	0.2200	0.6515	0.1769
16,38	-3.88 × 10 ⁻⁴	7.98 × 10 ⁻⁵	0.067	0.454	0.122	6.00 × 10 ⁻⁴	-1.80 × 10 ⁻⁴	0.0164	0.1648	1.6510
18,38	-3.19 × 10 ⁻⁴	6.78 × 10 ⁻⁵	0.125	0.155	0.530	5.43 × 10 ⁻⁴	-1.30 × 10 ⁻⁴	0.2081	0.6032	0.2423
20,38	-2.66 × 10 ⁻⁴	5.77 × 10 ⁻⁵	0.192	0.394	0.519	4.87 × 10 ⁻⁴	-1.40 × 10 ⁻⁴	0.0703	1.0250	0.1176
22,38	-2.01 × 10 ⁻⁴	6.23 × 10 ⁻⁵	0.446	0.167	0.062	4.45 × 10 ⁻⁴	-1.30 × 10 ⁻⁴	0.1268	0.1135	0.9652
24,38	-1.70 × 10 ⁻⁴	5.13 × 10 ⁻⁵	0.592	0.160	0.236	4.12 × 10 ⁻⁴	-1.00 × 10 ⁻⁴	0.7036	0.0758	0.9911
26,38	-1.36 × 10 ⁻⁴	4.81 × 10 ⁻⁵	0.520	0.149	0.238	3.72 × 10 ⁻⁴	-1.40 × 10 ⁻⁴	1.0600	0.1641	0.0506
28,38	-9.91 × 10 ⁻⁵	4.71 × 10 ⁻⁵	0.137	0.104	0.697	3.53 × 10 ⁻⁴	-9.63 × 10 ⁻⁵	0.9850	0.0786	0.7406
30,38	-7.08 × 10 ⁻⁵	4.83 × 10 ⁻⁵	0.074	1.680	0.020	3.33 × 10 ⁻⁴	-1.37 × 10 ⁻⁴	0.0448	0.8221	0.2001

In this VTPR equation, H₂S and CO₂ compounds which are entered as a database for searching the parameters have a small deviation from the modeling when Tr is below 1. The largest deviation in this study occurred in N₂. This can be seen in Fig. 3 in which at a reduced temperature below 1, N₂ appears to have larger deviations than other compounds such as H₂S and CO₂. In the area near Tr = 1 with the pressure of 12.38 MPa – 30.38 MPa, CO₂ and H₂S compounds appear to have larger deviations than other compounds in sour natural gas. These are shown in Fig. 3. When applying equations (10) and (11) and parameters in Table 4, the estimated volume of CO₂ and H₂S compounds produces %AAD which is higher than the %AAD of PR equation. The involvement of molecular weight and acentric factor in this translation equation gives high relative error when the CO₂ and H₂S are entered into the database, especially when approaching the critical temperature. Therefore, specifically for CO₂ and H₂S compounds, equation (12) is used to obtain the smaller %AAD VTPR. N₂ although overall has %AAD VTPR which is smaller than %AAD PR when using equation (10), better results are obtained using equation (12).

$$c = \frac{1}{M\omega} (C_1 + C_2 \cdot T_r) \quad (12)$$



(a)



(b)

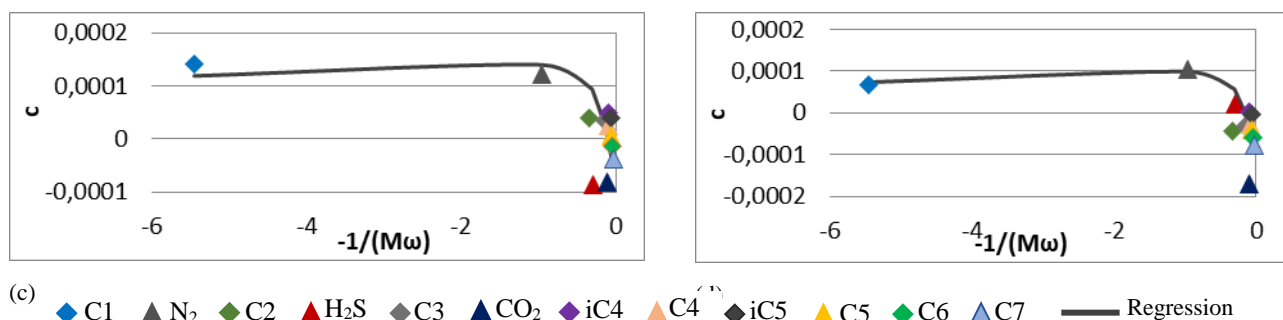


Figure 3: Parameter Optimization of VTPR as a Function of Molecular Weight and Acentric Factor of Each Pure Compound in Sour Natural Gas (a) $P = 12.38$ MPa, $T_r = 0.8$ (b) $P = 12.38$ MPa, $T_r = 0.95$ (c) $P = 12.38$ MPa, $T_r = 1.02$ (d) $P = 12.38$ MPa, $T_r = 1.08$

The volume translation values for each isotherm with the analyzed sour natural gas compounds were plotted against T_r and expressed as a linear function. The correlation equation for the VTPR equation parameters was developed as a function of molecular weight (M) and acentric factor (ω). Correlating $(M\omega)^{-1}$ with equation parameters gives a better result than VTPR as a function of molecular weight analyzed in this study. The estimation of CO_2 and H_2S volume with VTPR resulted in %AAD which was higher than 2% at $T_r = 0.8 - 1.08$ and pressure 12.38 MPa – 30.38 MPa. In the area above the critical temperature with a pressure of 12.38 MPa – 30.38 MPa, CO_2 and H_2S compounds appear to have larger deviations than other compounds in sour natural gas. Several linear temperature-dependent volume translation models have been developed to improve volume estimation only under subcritical conditions, and may not be suitable to be used in volume estimation in several above and below critical conditions^[10]. Discontinuity in the value of the volume shift can occur due to changes from the gas phase to the liquid phase^[17]. To improve the volume estimation near or higher than the critical region, more complex volume translation methods such as temperature-dependent volume translation with exponential equation models are formulated^[17].

4.3. VTPR as a Function of Acentric Factor

Previous research formulated the temperature-dependent VTPR equation as a function of the acentric factor (ω) as well^[11]. In this study, the equation was slightly modified to become equation (13). Nonlinear regression is applied to determine the equation parameters in which the equation is temperature-dependent. Three parameters (C_1 , C_2 , and C_3) obtained by regression were correlated with the specific properties of each compound which is the acentric factor (ω). The optimization values of C_1 , C_2 , and C_3 were carried out for various pure compounds in analyzed sour natural gas with temperature conditions ranging from $T_r = 0.8 - 1.08$. Parameter values (k_1 , k_2 , k_3 , k_4 , k_5 , and k_6) in equations (14)–(16), which are shown in Table 5, were optimized by linear regression and applied to the pressure of 12.38 MPa – 30.38 MPa. This optimization is applied to obtain the optimum parameter value with a small volume deviation.

$$c(T_r) = \frac{z_c R T_c}{P_c} \left\{ C_1 \exp \left[-\frac{(T_r - 1)^2}{2C_2^2} \right] + C_3 T_r \right\} \quad (13)$$

$$C_1 = k_1 \omega + k_2 \quad (14)$$

$$C_2 = k_3 \omega + k_4 \quad (15)$$

$$C_3 = k_5 \omega + k_6 \quad (16)$$

The volume estimated by using VTPR with translation equation as a function of acentric factor produces lower %AAD than the %AAD of the PR equation. The comparison of the volume estimation deviation by PR equation with the volume estimation by VTPR equation for each compound in the range of $T_r = 0.8 - 1.08$ and $P = 12.38 - 30.38$ MPa is shown in Table 3. Exponential VTPR with parameters as a function of ω has a lower deviation value than the other

two analyzed VTPR equations. This exponential equation also allows ω to be regressed with a low relative error which is shown in Fig. 4. The accuracy happens because the VTPR equation involves critical compressibility factor (Z_c) which is adjusted for each compound and the relationship between the VTPR parameter and ω which has a linear relationship with a small relative error

Table 5: Translation Equation Parameters as a Function of Acentric Factor

Pressure	k ₁	k ₂	k ₃	k ₄	k ₅	k ₆
12.38 MPa	0.14729	0.14199	-0.058279	0.4178	-0.22531	-0.11942
14.38 MPa	-0.21859	0.20174	-0.39189	0.5172	0.11931	-0.17211
16.38 MPa	-0.23841	0.17718	-0.47019	0.53653	0.14066	-0.14378
18.38 MPa	-0.22722	0.15168	-0.57329	0.5609	0.13036	-0.11528
20.38 MPa	-0.21649	0.13205	-0.69213	0.58567	0.1206	-0.093344
22.38 MPa	-0.20921	0.11723	-0.8122	0.60895	0.11439	-0.076724
24.38 MPa	-0.20337	0.10559	-0.94934	0.63432	0.10953	-0.063626
26.38 MPa	-0.1995	0.096453	-1.0921	0.65685	0.10663	-0.053313
28.38 MPa	-0.19617	0.088935	-1.1162	0.66161	0.10402	-0.044813
30.38 MPa	-0.19219	0.082492	-1.3527	0.70601	0.10102	-0.03762

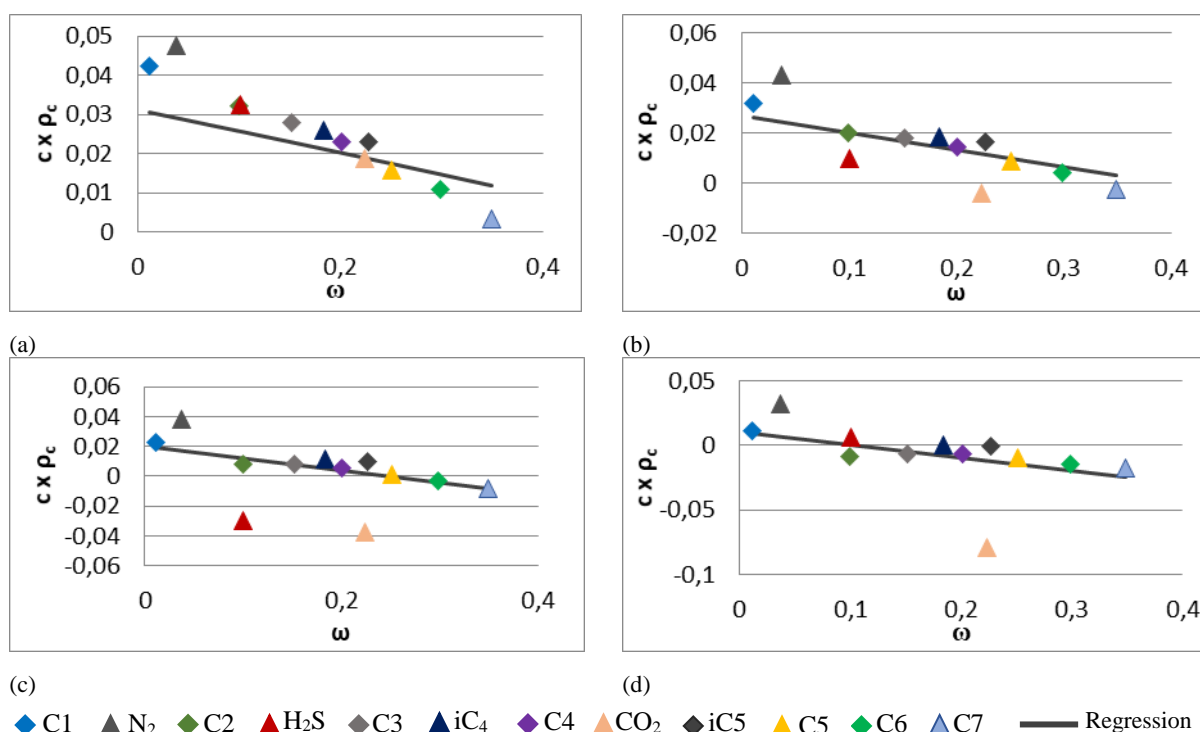


Figure 4: Parameter Optimization of VTPR as a Function of Acentric Factor of Each Pure Compound in Sour Natural Gas (a) $P = 12.38$ MPa, $T_r = 0.8$ (b) $P = 12.38$ MPa, $T_r = 0.95$ (c) $P = 12.38$ MPa, $T_r = 1.02$ (d) $P = 12.38$ MPa, $T_r = 1.08$

4.3. VTPR and Mixing Rule Application in Volume Estimation of Sour Natural Gas

The translation equation is also included in the mixing rule for mixed compounds volume estimation as shown in equations (17)-(19). In equation (17), c_m is the volume translation constant of the mixture, while x_i and c_i are the mole fraction and volume translation constant of each i pure compound in the mixture. The c_i value is obtained by using

equation (6) – (16) and the optimized parameters. Parameters a and b are the parameters contained in PR equation. The binary interaction parameter (K_{ij}) was obtained by optimizing several K_{ij} values for each of the two compounds contained in sour natural gas. In this study the composition of sour natural gas as a fixed variable, temperature and pressure as independent variables, and volume as the dependent variable. The composition of sour natural gas analyzed in this study is based on well P which is shown in Table 1. The deviations of the three VTPR and the mixing rule methods are shown in Table 6. The satisfying results in Table 6 show that the combination of VTPR and mixing rule can be recommended to estimate the volume of sour natural gas at 12.38 – 30.38 MPa and 315.37 - 360.37 K.

$$c_m = \sum_i c_i x_i \quad (17)$$

$$b_m = \sum_j x_j b_j \quad (18)$$

$$a_m = \sum_i \sum_j x_i x_j (1 - K_{ij}) a_i^{\frac{1}{2}} a_j^{\frac{1}{2}} \quad (19)$$

Table 6: Volume Deviation with VTPR and Mixing Rule

T (K)	P (MPa)	%AAD of VTPR as a function of M	%AAD of VTPR as a function of M and ω	%AAD of VTPR as a function of ω
335.37	12.38	0.00578%	0.00002%	0.00000%
335.37	14.38	0.00032%	0.00000%	0.00003%
335.37	16.38	0.00108%	0.00000%	0.00000%
335.37	18.38	0.00000%	0.00000%	0.00002%
335.37	20.38	0.00000%	0.00000%	0.00000%
335.37	22.38	0.00000%	0.00001%	0.00004%
335.37	24.38	0.00000%	0.00001%	0.00000%
335.37	26.38	0.00000%	0.00000%	0.00000%
335.37	28.38	0.00000%	0.00001%	0.00000%
335.37	30.38	0.00000%	0.00001%	0.00003%
315.37	20.38	0.00000%	0.00152%	0.00000%
320.37	20.38	0.00004%	0.00003%	0.00000%
325.37	20.38	0.00000%	0.00000%	0.00005%
330.37	20.38	0.00000%	0.00002%	0.00000%
335.37	20.38	0.00000%	0.00000%	0.00000%
340.37	20.38	0.00000%	0.00001%	0.00001%
345.37	20.38	0.00000%	0.00001%	0.00000%
350.37	20.38	0.00000%	0.00000%	0.00000%
355.37	20.38	0.00000%	0.00000%	0.00000%
360.37	20.38	0.00000%	0.00000%	0.00000%
%AAD Total		0.03618%	0.00825%	0.00097%

5. Conclusion

VTPR equations which parameters are a function of molecular weight, acentric factor function, and both estimate the volume of pure compounds in sour natural gas with %AAD 2.07%, 1.05%, and 1.47% respectively smaller than %AAD PR. Using the three respective VTPR methods and mixing rules, volume estimation of sour natural gas mixture gives %AAD 0.03618%, 0.00097%, 0.00825%, respectively. It can be concluded that these VTPR could provide accurate sour natural gas volume estimation. The VTPR equation which depends on temperature and as a

function of molecular weight results in poor volumetric estimation than other VTPR for pure components around the critical temperature especially at $T_r = 0.8 - 1.08$ for sour natural gas. CO_2 and H_2S compounds gave high %AAD because compared to other analyzed hydrocarbon compounds, H_2S and CO_2 have critical pressure (P_c) close to the pressure analyzed in this study. The linear VTPR equation which depends on temperature and as a function of molecular weight and acentric factor gives a better result than VTPR as a function of molecular weight. In the region near the critical temperature, CO_2 and H_2S compounds appear to have larger deviations than other compounds in sour natural gas. Several linear temperature-dependent VTPR might improve volume estimation at the subcritical condition, but might not be suitable in above and below the critical condition. Volume estimation has better accuracy with VTPR as a function of the acentric factor than the other two VTPR due to the exponential mathematical equation which involves Z_c . This exponential equation allows acentric factors to be regressed with a low relative error. The accuracy of the estimation of sour natural gas compounds is also caused by the adjustment of the Z_c value of each compound.

References

- [1] IEA, "Gas Market Report 2019 - Analysis and forecast to 2024," in "Demand," International Energy Agency, Paris, 2019. [Online]. Available: <https://www.iea.org/reports/gas-2019>
- [2] L. Xijia, P. Miles, F. Brock, and M. Mike, "A Novel Power Generation System Utilizing Un-treated Sour Gas Fuel," in *Abu Dhabi International Petroleum Exhibition & Conference*, 2018, vol. Day 1 Mon, November 12, 2018, D012S112R001, doi: 10.2118/192823-ms. [Online]. Available: <https://doi.org/10.2118/192823-MS>
- [3] D. Gong, S. Huang, W. Wu, C. Yu, C. Fang, and D. Liu, "Characteristics of gas compositions in giant gas fields of China," *Energy exploration & exploitation*, vol. 32, no. 4, pp. 635-656, 2014.
- [4] N. Azizi, R. Behbahani, and M. Isazadeh, "An efficient correlation for calculating compressibility factor of natural gases," *Journal of Natural Gas Chemistry*, vol. 19, no. 6, pp. 642-645, 2010.
- [5] J. Obuba, S. Ikiesnkimama, C. Ubani, and I. Ekeke, "Natural gas compressibility factor correlation evaluation for niger delta gas fields," *IOSR-JEEE*, vol. 6, no. 4, p. 10, 2013.
- [6] T. Ahmed, *Reservoir engineering handbook*. Gulf Professional Publishing, 2018.
- [7] J. G. Speight, "Chapter 4 - Corrosion in Gas Processing Plants," in *Oil and Gas Corrosion Prevention*, J. G. Speight Ed. Boston: Gulf Professional Publishing, 2014, pp. 67-91.
- [8] I. Ashour, N. Al-Rawahi, A. Fatemi, and G. Vakili-Nezhaad, "Applications of equations of state in the oil and gas industry," *Thermodynamics-Kinetics of Dynamic Systems*, vol. 7, pp. 165-178, 2011.
- [9] B. S. Jhaveri and G. K. Youngren, "Three-Parameter Modification of the Peng-Robinson Equation of State To Improve Volumetric Predictions," *SPE-13118-PA*, vol. 3, no. 03, pp. 1033-1040, 1988/8/1/ 1988, doi: 10.2118/13118-PA.
- [10] H. Baled *et al.*, "Prediction of hydrocarbon densities at extreme conditions using volume-translated SRK and PR equations of state fit to high temperature, high pressure PVT data," *Fluid Phase Equilibria*, vol. 317, pp. 65-76, 2012.
- [11] J. Shi, H. A. Li, and W. Pang, "An improved volume translation strategy for PR EOS without crossover issue," *Fluid Phase Equilibria*, vol. 470, pp. 164-175, 2018/08/25/ 2018, doi: <https://doi.org/10.1016/j.fluid.2018.01.034>.
- [12] D.-Y. Peng and D. B. Robinson, "A new two-constant equation of state," *Industrial & Engineering Chemistry Fundamentals*, vol. 15, no. 1, pp. 59-64, 1976.
- [13] A. M. Abudour, S. A. Mohammad, R. L. Robinson, and K. A. M. Gasem, "Volume-translated Peng–Robinson equation of state for saturated and single-phase liquid densities," *Fluid Phase Equilibria*, vol. 335, pp. 74-87, 2012/12/15/ 2012, doi: <https://doi.org/10.1016/j.fluid.2012.08.013>.

- [14] M. Nazarzadeh and M. Moshfeghian, "New volume translated PR equation of state for pure compounds and gas condensate systems," *Fluid Phase Equilibria*, vol. 337, pp. 214-223, 2013/01/15/ 2013, doi: <https://doi.org/10.1016/j.fluid.2012.10.003>.
- [15] A. Péneloux, E. Rauzy, and R. Fréze, "A consistent correction for Redlich-Kwong-Soave volumes," *Fluid phase equilibria*, vol. 8, no. 1, pp. 7-23, 1982.
- [16] K. Frey, "Improving Thermodynamic Property Estimation through Volume Translation," Doctor of Science in Chemical Engineering, Department of Chemical Engineering, Massachusetts Institute of Technology, 2005.
- [17] J. Shi and H. A. Li, "Criterion for determining crossover phenomenon in volume-translated equation of states," *Fluid Phase Equilibria*, vol. 430, pp. 1-12, 2016.