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QUANTITATIVE ASSESSMENT OF A NOVEL METHOD FOR FLUID THERMODYNAMIC TEST SIMULATION IN MULTICOMPONENT SYSTEMS

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Summary

This paper presents a quantitative methodology for simulating fluid thermodynamic tests, including constant composition expansion (CCE), differential liberation (DL), and separator tests, within multicomponent systems. The approach combines equilibrium ratios, flash calculations, and the Peng-Robinson equation of state. Utilizing the PVTp (Pressure - Volume - Temperature) package regression procedure enables the calibration of OmegaA and OmegaB values, enhancing accuracy and minimizing error margins in fluid thermodynamic calculations compared to empirical data. Numerical results demonstrate the effectiveness of this method. Bubble point pressure values from observed, software-generated, and calculated data are 2344, 2339, and 2350.42 psia, respectively. Calculated fluid thermodynamic test results closely align with software predictions and exhibit acceptable error levels compared to the measured data. However, discrepancies in the solution gas - oil ratio during the DL test highlight the need for more comprehensive measured data to improve simulation accuracy and reduce error margins. The comparison between the proposed methodology and collected data confirms the effectiveness of integrating equilibrium ratios, flash calculations, and the Peng-Robinson equation of state for precise fluid thermodynamic calculations. This approach offers a quantitative framework for simulating fluid thermodynamic tests, providing insights while reducing reliance on costly laboratory experiments.

Key words: Fluid thermodynamic tests, CCE test, DL test, separator test, equilibrium ratio, flash calculation, Peng-Robinson EOS.

1. Introduction

In the realm of reservoir engineering, the composition of reservoir fluids varies widely, encompassing a diverse array of hydrocarbons and non-hydrocarbons, thereby introducing significant chemical complexity. To address this complexity and gain insights into the phase behavior of such intricate fluids, equations of state have emerged as valuable tools. These equations establish precise mathematical relationships between pressure, volume, and temperature, enabling the comprehensive modeling of volumetric characteristics, vapor - liquid equilibria, and thermal properties, both for pure substances and complex mixtures [1].

In the field of petroleum engineering, the application of equations of state is a common practice in the computation of various tests, including the constant composition expansion (CCE), differential liberation (DL), and separator tests [2]. These tests serve as indispensable tools for elucidating volumetric behavior, vapor - liquid equilibria, and thermal properties of reservoir fluids. Typically, conducting these tests in a laboratory necessitates the use of expensive PVT (pressure - volume - temperature) equipment and the expertise of skilled personnel [3, 5]. However, the application of an equation of state offers a compelling alternative by enabling the simulation of these tests based on specific hydrocarbon composition data, thus providing a cost-effective and efficient means to glean valuable insights [6].

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2. Methodology

2.1. Laboratory thermodynamic test for multi-component hydrocarbon system

2.1.1. Principle of constant composition expansion test

Constant composition expansion experiments on gas condensates or crude oil are carried out to replicate the pressure - volume relationships of these hydrocarbon systems. The test is performed to determine:

- Saturation pressure (bubble point or dew point pressure).

- Single-phase fluid isothermal compressibility coefficients in excess of saturation pressure...

The ratio of the reference volume signifies the hydrocarbon system's volume in relation to the cell pressure. This critical parameter is known as the relative volume and can be expressed mathematically as follows [1]:

$$V_{rel} = \frac{V_t}{V_{sat}} \tag{1}$$

Where:

V_{rel}: Relative volume

V_t: Total hydrocarbon volume

V_{sat}: Volume at the saturation pressure

At saturation pressure, the relative volume is equal to 1. This test is also known as flash liberation, flash vaporization, or flash expansion.

It should be emphasized that no hydrocarbon material is taken from the cell; therefore, the composition of the overall hydrocarbon mixture in the cell stays constant.

The density of the oil may be determined above the bubble point pressure using the observed relative volume:

$$\rho = \frac{\rho_{sat}}{V_{rel}} \tag{2}$$

Where

ρ: Density at any pressure above the saturation pressure

ρ_{sat}: Density at the saturation pressure

V_{rel} : Relative volume

Smoothing is commonly required to adjust laboratory mistakes in estimating total hydrocarbon volume immediately below saturation pressure and at lower pressures. To smooth the values of the relative volume, a dimensionless compressibility function, also known as the Y-function, is utilized. In its mathematical form, the function is only defined below the saturation pressure and represented by the expression:

$$Y = \frac{p_{sat} - p}{p(V_{rel})} \tag{3}$$

The Y-function, displayed on a Cartesian scale as a function of pressure, effectively smooths relative volume data below saturation pressure. Graphically, the Y-function typically appears as a straight line or exhibits slight curvature. The following steps outline the simple process for smoothing and correcting relative volume data [1]:

Step 1: Utilizing equation (3), compute the Y-function values for all pressures falling below the saturation pressure.

Step 2: On a Cartesian scale, construct a plot illustrating the relationship between the Y-function and pressure.

Step 3: Determine the coefficients for the best-fit line, expressed as:

$$Y = a + bp \tag{4}$$

Here, 'a' and 'b' correspond to the intercept and slope of the linear regression, respectively.

Step 4: Re-evaluate the relative volume at all pressures below the saturation point using the Expression (5):

$$V_{rel} = 1 + \frac{p_{sat} + p}{p(a + bp)} \tag{5}$$

Isothermal compressibility coefficients are used to solve numerous reservoir engineering problems, including transient fluid flow difficulties, and to determine the physical parameters of undersaturated crude oil.

The isothermal compressibility (c) of a material can be precisely described through the mathematical expression:

$$c = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T \tag{6}$$

To calculate the isothermal compressibility coefficient (c_o) for the oil phase above the bubble point, you can use one of these equivalent equations:

$$c_o = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T \tag{7}$$

$$c_o = -\frac{1}{B_o}\left(\frac{\partial B_o}{\partial p}\right)_T \tag{8}$$

$$c_o = -\frac{1}{\rho_o}\left(\frac{\partial \rho_o}{\partial p}\right)_T \quad (9)$$

$$c_o = \frac{-1}{B_o}\frac{\partial B_o}{\partial p} + \frac{B_g}{B_o}\frac{\partial R_s}{\partial p} \quad (10)$$

Where:

c_o: Isothermal compressibility

B_o: Oil formation volume factor

B_g: Gas formation volume factor

T: Temperature

p: Pressure

Equations (6) - (10) define oil compressibility, which may be expressed in terms of relative volume as:

$$c_o = -\frac{1}{V_{rel}}\frac{\partial V_{rel}}{\partial p} \quad (11)$$

The relative volume above the bubble point pressure is commonly displayed as a function of pressure. To evaluate c_o at any pressure p, all that is required is to draw a tangent line and determine the slope of the line, i.e. $\frac{\partial V_{rel}}{\partial p}$,

It should be noticed that it lists the compressibility coefficient at various pressure levels. These values are calculated by computing the changes in relative volume at the specified pressure intervals and assessing the relative volume at the lower pressure, or

$$c_o = \frac{-1}{[V_{rel}]_2}\frac{(V_{rel})_1 - (V_{rel})_2}{p_1 - p_2} \quad (12)$$

with the subscripts 1 and 2 demonstrating the values at the higher and lower pressure ranges, respectively.

2.1.2. Principle of Differential Liberation (DL) test

The solution gas liberated from an oil sample during a pressure drop is constantly removed from contact with the oil before achieving equilibrium with the liquid phase in the differential liberation process. The overall hydrocarbon system's composition varies during this sort of escape. The test produced the following experimental outcomes:

- Gas concentration in solution is a function of pressure.

- Oil volume shrinkage is a function of pressure.

- Properties of the evolved gas, such as the composition of the liberated gas, the gas compressibility factor, and the gas-specific gravity.

- The remaining oil's density is a function of pressure.

The differential liberation test is thought to better represent the separation process occurring in the reservoir and to model the flowing behavior of hydrocarbon systems above the critical gas saturation. When the saturation of the liberated gas reaches the critical value, it begins to flow, leaving behind the oil that initially housed it. This is due to the fact that gasses have better mobility than oils in general. As a result, this behavior is consistent with the differential liberation sequence [1].

2.1.3. Principle of separator test

Separator tests are performed to examine how the volumetric behavior of reservoir fluid changes as it flows through the separator (or separators) and into the stock tank. The resultant volumetric behavior is heavily impacted by the surface separation facilities' working parameters, such as pressures and temperatures. The main objective of conducting separator tests is to give the critical laboratory information required to determine the appropriate surface separation conditions that will enhance stock-tank oil output. Furthermore, when the test findings are properly integrated with the differential liberation test data, they give a method of getting the PVT parameters (B_o, R_s, and B_t) necessary for petroleum engineering calculations. Only the original oil at the bubble point is used in these separation tests [1].

2.2. Equilibrium ratios and flash calculation

2.2.1. Equilibrium ratio for ideal gas

In the context of multicomponent systems, the equilibrium ratio K_i is established as the ratio of a component's mole fraction in the gas phase (y_i) to its mole fraction in the liquid phase (x_i). This mathematical relationship is formally expressed as follows [2]:

$$K_i = \frac{y_i}{x_i} \quad (13)$$

For pressures below 100 psia, Raoult's and Dalton's laws provide a simple way to calculate equilibrium ratios. Raoult's law states that the partial pressure (P_i) of a component in a multicomponent system is the product of its mole fraction in the liquid phase (x_i) and its vapor pressure (P_{vi}).

$$p_i = x_i p_{vi} \quad (14)$$

Conversely, Dalton's law states that the partial pressure of a component is calculated by multiplying its mole fraction in the gas phase (y_i) by the total pressure of the system (P):

$$p_i = y_i p \tag{15}$$

Where 'p' represents the total system pressure in psi.

At a state of equilibrium, in accordance with the aforementioned principles, the partial pressure exerted by a component in the gas phase is required to be equal to the partial pressure exerted by the same component in the liquid phase. Combining the equations that characterise these two fundamental laws yields the expression:

$$x_i p_{vi} = y_i p \tag{16}$$

Upon rearranging this relationship and incorporating the concept of the equilibrium ratio, the equation can be reformulated as follows:

$$\frac{y_i}{x_i} = \frac{p_{vi}}{p} = K_i \tag{17}$$

For ideal solutions, the equilibrium ratio depends only on system pressure (p) and temperature (T) regardless of the overall composition of the hydrocarbon mixture since the vapor pressure of a component is solely temperature-dependent.

The total number of moles in the system is defined as:

$$n = n_L + n_V \tag{18}$$

Where 'n' represents the total number of moles in the system, 'n_L' is the total number of moles in the liquid phase, and 'n_V' denotes the total number of moles in the vapor phase.

Consequently, a material balance on the ith component can be expressed as:

$$z_i n = x_i n_L + y_i n_V \tag{19}$$

Where: z_i: Mole fraction of component in the entire hydrocarbon mixture

Furthermore, by utilizing the concept of mole fraction, we can articulate the equation as:

$$\begin{gathered}\sum_i x_i = 1\\ \sum_i y_i = 1\\ \sum_i z_i = 1\end{gathered} \tag{20}$$

All phase-equilibria calculations may be performed based on 1 mol of the hydrocarbon mixture, i.e., n = 1. This assumption is reduced to

$$n_L + n_V = 1 \tag{21}$$

$$x_i n_L + y_i n_V = z_i \tag{22}$$

Combining equations (21) and (22) to exclude y_i results in

$$x_i n_L + (x_i K_i) n_V = z_i \tag{23}$$

When we solve for x_i, we get

$$x_i = \frac{z_i}{n_L + K_i n_V} \tag{24}$$

It is also possible to solve it for y_i by combining to delete x_i:

$$y_i = \frac{z_i K_i}{n_L + K_i n_V} = x_i K_i \tag{25}$$

When all of the equations are combined, the result is

$$\sum_i x_i = \sum_i \frac{z_i}{n_L + K_i n_V} = 1 \tag{26}$$

and

$$\sum_i y_i = \sum_i \frac{z_i K_i}{n_L + K_i n_V} = 1 \tag{27}$$

Since

$$\sum_i y_i - \sum_i x_i = 0 \tag{28}$$

therefore

$$\sum_i \frac{z_i K_i}{n_L + K_i n_V} - \sum_i \frac{z_i}{n_L + K_i n_V} = 0 \tag{29}$$

or

$$\sum_i \frac{z_i (K_i - 1)}{n_L + K_i n_V} = 0 \tag{30}$$

When is replaced with (1 - n_V), the result is

$$f(n_V) = \sum_i \frac{z_i (K_i - 1)}{n_V (K_i - 1) + 1} = 0 \tag{31}$$

This compilation of equations furnishes the essential phase relationships necessary for conducting volumetric and compositional assessments of hydrocarbon systems. Such calculations, as denoted in the scientific literature, are commonly referred to as "flash calculations" [2].

2.2.2. Equilibrium ratio for real gas

The equilibrium ratios, as discussed in Section 2.2.1, which describe the distribution of each component between the liquid and gas phases in terms of vapor pressure and system pressure, have been found to be insufficient. This deficiency arises from certain critical assumptions, namely:

- The ideal gas assumption characterizes the vapor phase according to Dalton's law.

- The ideal solution assumption characterizes the liquid phase as stipulated by Raoult's law.

At elevated pressures, these assumptions break down, leading to imprecise equilibrium ratio calculations. In a realistic solution, these ratios are no longer exclusively dependent on pressure and temperature but are also influenced by the composition of the hydrocarbon mixture. This concept can be quantified as follows:

$$K_i = K(P,T,z_i)$$

Various methods have been proposed for determining equilibrium ratios in hydrocarbon mixtures. These correlations span a spectrum, from fundamental mathematical expressions to complex equations involving multiple composition-dependent variables.

Notably, Wilson (1968) devised a concise thermodynamic formulation for computing K values, articulated as follows [2]:

$$K_i = \frac{p_{ci}}{p} exp\,[5.37(1 + \omega_i)(1 - \frac{T_{ci}}{T})] \tag{32}$$

Where:

P_{ci}: Critical pressure of component i

T_{ci}: Critical temperature of component i

ω_i : Acentric factor of component i

When applied under low pressure conditions, this equation yields more accurate equilibrium ratio values.

2.2.3. Flash calculation

All reservoir and process engineering calculations include flash calculations. They are required to determine the amount (in moles) of hydrocarbon liquid and gas coexisting in a reservoir or vessel at a specific pressure and temperature. These computations are also necessary to determine the composition of the present hydrocarbon stages. Flash calculations are used to calculate the moles of the gas phase, n_V, moles of the liquid phase, n_L, liquid phase composition, x_i, and gas phase composition, y_i, given the total composition of a hydrocarbon system at a certain pressure and temperature [2].

The following stages outline the computational methods for finding n_L, n_V, y_i, and x_i of a hydrocarbon mixture with a known overall composition of z_i and defined by a set of equilibrium ratios, K_i.

The first step involves using the Newton-Raphson iterative approach to determine n_V, following these iterative procedures [2]:

Beginning with an arbitrary value assumption for n_V, for instance, $n_V = 0.5$, the following relation is used to calculate an improved assumed value [2]:

$$n_V = \frac{A}{A + B} \tag{33}$$

with

$$A = \sum_i [z_i(K_i - 1)]$$

$$B = \sum_i [z_i(\frac{1}{K_i} - 1)]$$

When contemplating the correctness of the equilibrium ratios, these equations hold the potential to yield an initial estimation for n_V. It is imperative to emphasize that the ascribed value for n_V must adhere to the constraints $0 < n_V < 1$.

In accordance with the adopted, preliminary n_V value, the function $f(n_V)$ is defined:

$$f(n_V) = \sum_i \frac{z_i(K_i - 1)}{n_V(K_i - 1) + 1} = 0$$

When the magnitude of the function $f(n_V)$ falls below a predefined threshold, typically set at values like 10^{-6}, the initially assumed value of n_V serves as the sought-after solution.

However, in cases where the absolute value of $f(n_V)$ surpasses the predetermined tolerance, an updated value, denoted as (n_V)_new, is determined via the subsequent expression:

$$(n_V)_{new} = n_V - \frac{f(n_V)}{f'(n_V)} \tag{34}$$

using the derivative $f'(n_V)$ defined by

$$f'(n_V) = -\sum_i \{\frac{z_i(K_i - 1)^2}{[n_V(K_i - 1) + 1]^2}\} \tag{35}$$

And $(n_V)_{new}$ is the new n_V value that will be utilized in the following iteration. This operation is continued with each new value of n_V until convergence is reached, i.e.

$$|f(n_V)| \le \varepsilon$$

Or

$$|(n_V)_{new} - n_V| \le \varepsilon$$

Where:

ϵ: Preset error tolerance

When convergence is reached, n_L, x_i, y_i are derived.

2.3. Peng-Robinson equation of state & its applications

2.3.1. Fundamental of Peng-Robinson equation of state

Peng and Robinson are engaged in an extensive research endeavor aimed at evaluating the applicability of the Soave-Redlich-Kwong (SRK) equation of state in forecasting the characteristics of naturally transpiring hydrocarbon systems. Their investigations have illuminated the necessity for enhancing the equation of state's capability to anticipate various fluid properties, with a specific emphasis on liquid densities, particularly within the critical region. In pursuit of this objective, Peng and Robinson posited the subsequent formula as an initial framework for the development of an enhanced predictive model [1]:

$$p = \frac{RT}{V - b} - \frac{a\alpha}{V(V + b) + b(V - b)} \tag{36}$$

The traditional critical point conditions are enforced, and the parameters a and b are calculated:

$$a = 0.45724\frac{R^2T_c^2}{P_c} \tag{37}$$

$$b = 0.07780\frac{RT_c}{P_c} \tag{38}$$

Peng and Robinson utilized Soave's approach to calculate the temperature-dependent parameter α:

$$\alpha = \left[1 + m\left(1 - \sqrt{\frac{T}{T_c}}\right)\right]^2 \tag{39}$$

at

$$m = 0.3796 + 1.54226\omega - 0.2699\omega^2 \tag{40}$$

The following adjusted equation for the m value is also offered for heavier components with acentric values $\omega > 0.49$:

$$m = 0.379642 + 1.48503\omega - 0.1644\omega^2 + 0.016667\omega^3 \tag{41}$$

It will provide the compressibility factor form Z if it is rearranged:

$$Z^3 - (B - 1)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \tag{42}$$

Using the thermodynamic connection, the following formula for the fugacity of a pure component can be obtained by:

$$\ln\left(\frac{f}{P}\right) = \ln(\phi) = Z - 1 - \ln(Z - B) - \left(\frac{A}{2\sqrt{2}B}\right)\ln\left(\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B}\right) \tag{43}$$

The following formula shows the fugacity coefficient of component i in a hydrocarbon liquid mixture:

$$\ln(\phi_i^L) = \frac{b_i(Z_L - 1)}{b_m} - \ln(Z_L - B) - \left(\frac{A}{2\sqrt{2}B}\right)\left[\frac{2\Psi_i}{(a\alpha)_m} - \frac{b_i}{b_m}\right]\ln\left(\frac{Z_L + (1 + \sqrt{2})B}{Z_L + (1 - \sqrt{2})B}\right) \tag{44}$$

Where b_m, B, A, Ψ_i, and $(a\alpha)_m$ are the previously established mixing parameters.

Any component's fugacity coefficient in the gas phase is computed by

$$\ln(\phi_i^V) = \frac{b_i(Z_V - 1)}{b_m} - \ln(Z_V - B) - \left(\frac{A}{2\sqrt{2}B}\right)\left[\frac{2\Psi_i}{(a\alpha)_m} - \frac{b_i}{b_m}\right]\ln\left(\frac{Z_V + (1 + \sqrt{2})B}{Z_V + (1 - \sqrt{2})B}\right) \tag{45}$$

Alternatively, the fugacity coefficient for any gas phase component is computed by substituting the liquid phase composition (x_i) with the gas phase composition (y_i) in the composition-dependent terms of the equation [1].

2.3.2. Applying the equation of state to determine equilibrium ratio

Upon satisfaction of all the specified conditions, the obtained solution is considered successful. In case that these criteria are not met, the sequence of steps denoted as steps 1 to 6 must be iteratively executed until the equilibrium ratios are found and confirmed. The process for ascertaining equilibrium ratios through the utilization of the equation of state is succinctly encapsulated in Figure 1.

2.3.3. Applications of the equation of state to calculate constant composition expansion (CCE) test

Step 1: Apply equation (24) in Section 2.2.1 to calculate x_i, y_i, n_L, n_V, K

Step 2: Determine the mixing parameters $(a\alpha)_m$ and b_m for the gas and liquid phases, resulting in:

- For the gas phase:

$$(a\alpha)_m = \sum_i\sum_j\left[y_iy_j\sqrt{a_ia_j\alpha_i\alpha_j}(1 - k_{ij})\right] \qquad b_m = \sum_i(y_ib_i) \tag{46}$$

- For the liquid phase:

$$(a\alpha)_m = \sum_i\sum_j\left[x_ix_j\sqrt{a_ia_j\alpha_i\alpha_j}(1 - k_{ij})\right] \qquad b_m = \sum_i(x_ib_i) \tag{47}$$

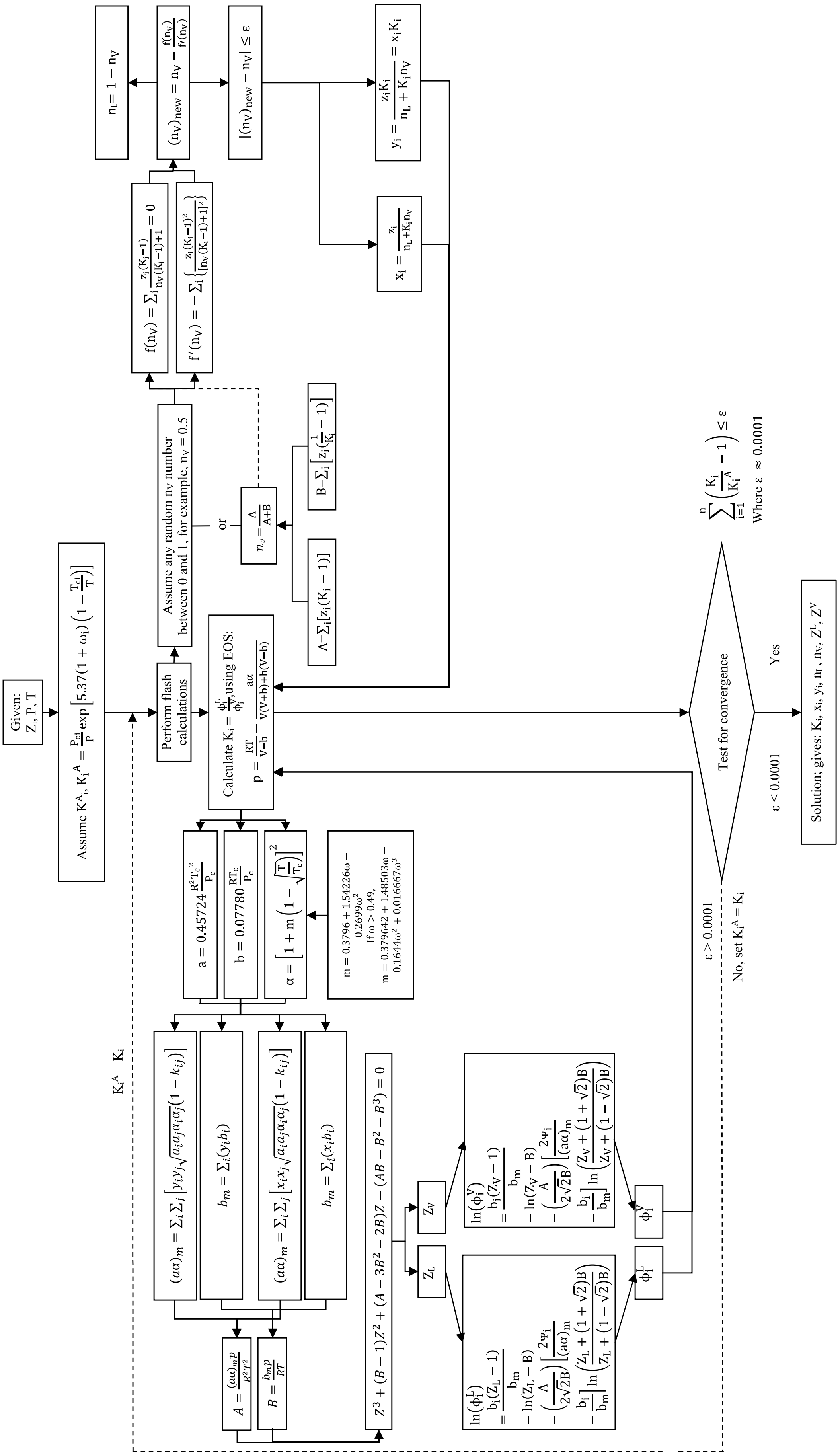

Figure 1. Flow diagram for determining equilibrium ratio using EOS [2].

Step 3: Calculate the coefficients A and B, for the gas/liquid phase, to give:

$$A = \frac{(a\alpha)_m p}{R^2 T^2} \quad (48)$$

$$B = \frac{b_m p}{RT} \quad (49)$$

Step 4: Determine the compressibility factor of the gas and liquid phases to yield:

$$Z^3 + (B - 1)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0 \quad (50)$$

- For the gas phase: Z_V
- For the liquid phase: Z_L

Step 5: Calculate the adjusted densities and specific gravities of both phases (ρ_V, ρ_L, γ_V, γ_L)

$$\rho = \frac{pM_a}{RTZ} \quad (51)$$

$$\gamma_V = \frac{\rho_V}{\rho_{air}} \quad (52)$$

$$\gamma_L = \frac{\rho_L}{\rho_{water}} \quad (53)$$

Step 6: Apply equation (1) to equation (12) in Section 2.1.1 to calculate V_g, V_L, V_o, c_o

Step 7: Calculate the relative total volume

The isothermal compressibility coefficient of a single-phase fluid is commonly calculated using the equation above the saturation pressure.

$$c_o = -\frac{1}{V_{rel}}\left(\frac{\partial V_{rel}}{\partial p}\right)_T \quad (54)$$

In addition to the previously obtained experimental data, the gas compressibility factor, Z, is found for gas - condensate systems.

Below saturation pressure, the two-phase volume, V_t, is represented as a percentage of the volume at saturation pressure.

$$Relative\ total\ volume = \frac{V_t}{V_{sat}} \quad (55)$$

With V_t is total hydrocarbon volume.

Because no hydrocarbon material is eliminated from the cell, the composition of the overall hydrocarbon mixture in the cell remains constant [1].

2.3.4. Applications of the equation of state to calculate differential liberation test [1]

Step 1: Calculate relative oil volume factor (B_o):

$$B_o = \frac{V_L}{V_{sc}} \quad (56)$$

at

$$V_L = \frac{n_L Z_L RT}{p} \quad (57)$$

Step 2: Calculate solution GOR (R_s):

$$R_s = \frac{V_{gsc}}{V_{stosc}} \quad (58)$$

Step 3: Calculate gas volume factor (B_g)

$$B_g = \frac{V_g}{V_{gsc}} \quad (59)$$

Step 4: Calculate two phase volume factors (B_t)

$$B_t = B_o + R_p B_g \quad (60)$$

2.3.5. Applications of the equation of state to calculate separator test

Step 1: Determine the amount of oil filled by one pound of crude at the reservoir pressure and temperature, which is designated V_o. Remembering and applying the equation that determines the number of moles:

$$n = \frac{m}{M_a} = \frac{\rho_o V_o}{M_a} = 1 \quad (61)$$

V_o is then derived by:

$$V_o = \frac{M_a}{\rho_o} \quad (62)$$

Step 2: Calculate the equilibrium ratios for the initial stream composition (z_i) entering the first separator and the separator's operating conditions, such as pressure and temperature.

Step 3: Utilizing the equilibrium ratios obtained in step 2 and assuming an initial feed of 1 mol entering the first separator, perform flash calculations to ascertain the gas and liquid compositions and quantities (in moles) leaving the initial separator. The quantities of gas and liquid exiting the first separation stage are referred to as $(n_L)_1$ and $(n_v)_1$, respectively.

$$[n_v]_1 = (n)(n_v)_1 = (1)(n_v)_1 \quad (63)$$

$$[n_L]_1 = (n)(n_L)_1 = (1)(n_L)_1 \quad (64)$$

Step 4: Calculate the equilibrium ratios for the liquid leaving the first separator, using its composition ($z_i = x_i$) as the input, at the operating pressure and temperature of the second separator.

Step 5: Begin with 1 mol of initial feed, conduct flash calculations to determine the gas and liquid compositions and quantities leaving the second separation stage. These calculations yield the precise number of moles for both gas and liquid phases.

$$[n_{v2}]_a = [n_{L1}]_a(n_v)_2 = (1)(n_L)_1(n_v)_2 \tag{65}$$

$$[n_{L2}]_a = [n_{L1}]_a(n_L)_2 = (1)(n_L)_1(n_L)_2 \tag{66}$$

Step 6: Repeat the preceding technique for each separation stage, including stock tank storage, and note the computed moles and compositions. The total number of moles of gas produced by all steps is then computed as follows:

$$(n_v)_t = \sum_{i=1}^{n}(n_{va})_i = (n_v)_1 + (n_L)_1(n_v)_2 + (n_L)_1(n_L)_2(n_v)_3 + \cdots + (n_L)_1 \ldots (n_L)_{n-1}(n_v)_n \tag{67}$$

The above expression can be expressed more succinctly:

$$(n_v)_t = (n_v)_1 + \sum_{i=2}^{n}\left[(n_v)_i \prod_{j=1}^{i-1}(n_L)_j\right] \tag{68}$$

Total moles of liquid left in the stock tank can alternatively be determined as follows:

$$(n_L)_{st} = n_{L1}\, n_{L2} \ldots n_{Ln} \tag{69}$$

or

$$(n_L)_{st} = \prod_{i=1}^{n}(n_L)_i \tag{70}$$

Step 7: Determine the volume (in scf) of all liberated solution gas from:

$$V_g = 379.4(n_v)_t \tag{71}$$

Step 8: Calculate the amount of stock tank oil occupied by $(n_L)_{st}$ moles of liquid using the following formula:

$$(V_o)_{st} = \frac{(n_L)_{st}(M_a)_{st}}{(\rho_o)_{st}} \tag{72}$$

Step 9: Using the following formulas, calculate the specific gravity and API gravity of the stock tank oil:

$$\gamma_o = \frac{(\rho_o)_{st}}{62.4} \tag{73}$$

$$°API = \frac{141.5}{\gamma_o} - 131.5 \tag{74}$$

Step 10: Determine the overall gas - oil ratio (also known as the gas solubility R_s):

$$GOR = \frac{V_g}{(V_o)_{st}/5.615} = \frac{(5.615)(379.4)(n_v)_t}{(n_L)_{st}\ (M)_{st}/(\rho_o)_{st}}$$

$$GOR = \frac{2130.331(n_v)_t(\rho_o)_{st}}{(n_L)_{st}(M)_{st}} \tag{75}$$

Step 11: Using the relationship, calculate the oil formation volume factor:

$$B_o = \frac{V_o}{(V_o)_{st}} \tag{76}$$

Combining equation (62) and equation (72) with the above expression gives:

$$B_o = \frac{M_a(\rho_o)_{st}}{\rho_o(n_L)_{st}(M_a)_{st}} \tag{77}$$

The separator pressure may be optimized by calculating the API gravity, GOR, and B_o at various assumed pressures as described above. The optimal pressure correlates to the highest API gravity and the lowest gas - oil ratio and oil formation volume factor [1].

3. Result and discussion

3.1. Overview of X oil field

The X oil field is situated within Block 01-X2, situated approximately 162 km off the northeastern coast of Ba Ria - Vung Tau province. This region is characterized by the development of several oil fields. Covering approximately 20.6 km^2 and residing at a water depth of approximately 43 m, the X oil field is operated under the product sharing agreement established between PVN and its partners. The oil field X was discovered in March 1996 when the exploration well A-1X was drilled for this purpose. Subsequently, three additional appraisal wells were drilled within the field to ascertain the in-situ reserves and the feasibility of reservoir exploitation within the terrigenous and basement sedimentary strata [5].

Recent well tests conducted at the A-4X well within the basement strata indicated a consistently favorable and robust oil flow at peak capacity. Commencing on April 17, 2011, the drilling of the A-4X has led to ongoing evaluations focused on on-site reserve estimation and recovery, marking a significant development in the field's operational progress.

3.2. Summary the data of the oil well XX-3Y

The methodology of employing lumping schemes has been adopted to condense the range of components, effectively reducing them from the C_{36+} group to the C_{12+} category. This strategic simplification of the component count is instrumental in streamlining the computational procedures, where the molecular weight of the C_{12+} group is 299.79 g/mol. Within this paradigm, distinct clusters of pure components are each substituted by a singular pseudo-component. These pseudo-components facilitate the application of mixing rules for the precise

Table 1. *Compositional data of the XX-3Y*

Component	Mole fraction	Component	Mole fraction	Component	Mole fraction
N_2	0	C_{10}	3.31	C_{24}	0.51
CO_2	0.34	C_{11}	3.05	C_{25}	0.55
H_2S	0	C_{12}	3.32	C_{26}	0.51
C_1	33.82	C_{13}	3.23	C_{27}	0.44
C_2	4.67	C_{14}	2.87	C_{28}	0.3
C_3	4.89	C_{15}	3.72	C_{29}	0.27
iC_4	1.25	C_{16}	2.47	C_{30}	0.31
nC_4	2.45	C_{17}	2.02	C_{31}	0.29
iC_5	0.96	C_{18}	2.2	C_{32}	0.29
nC_5	1.08	C_{19}	1.68	C_{33}	0.06
C_6	1.42	C_{20}	1.28	C_{34}	0.04
C_7	2.23	C_{21}	1.06	C_{35}	0.18
C_8	3.37	C_{22}	0.92	C36+	5.07
C_9	2.97	C_{23}	0.58		
MW $C_{36+} = 652.73$ g/mol, $\gamma = 0.872$					

Table 2. *Reservoir conditions of the XX- 3Y*

Reservoir pressure (psia)	4,495
Reservoir temperature (°F)	225.9

Table 3. *Sample study at reservoir temperature of the XX-3Y*

Bubble point pressure (psia)	2,344

Table 4. *Constant composition expansion at 225.9°F of the XX-3Y*

CCE test	Pressure (psia)	Relative volume ($V_r = V_t/V_b$)	Liquid density (kg/m^3)
p_b	2,344	1	701
	2,600	0.997	703
	2,800	0.995	705
	3,000	0.993	706
	3,300	0.99	708
	3,500	0.988	710
	3,700	0.986	711
	3,900	0.985	712
	4,100	0.983	714
	4,300	0.981	715
p_i	4,495	0.979	716

Table 5. *Separator test of the XX-3Y*

Separator test	Temperature (°F)	Pressure (psia)	GOR (scf/bbl)	Liq. Den (kg/m^3)	Oil FVF (B_o) (bbl/stb)
Stage 1	158	200	395	823	1,316
Tank	60	15	46	862	1

determination of essential EOS parameters, including critical pressure (p_c), critical temperature (T_c), and acentric factor (ω). These modified constants are subsequently assigned to the newly formed lumped pseudo-components, effectively enhancing the efficiency of the overall modeling process.

3.3. Regression & simulation of fluid thermodynamic tests workflow

3.3.1. Regression workflow by PVTp software

Step1: Choose a database from the PVTp option list including hydrocarbons, non-hydrocarbons, and pseudo components.

Table 6. *Differential liberation at 225.9°F- liquid properties of the XX-3Y*

DL test	Pressure (psia)	Oil FVF - B_o (bbl/stb)	Solution gas GOR R_s (scf/bbl)	Calculated liquid density (kg/m^3)
p_i	4,495	1,357	512	716
	4,300	1,359	512	715
	4,100	1,362	512	714
	3,900	1,364	512	712
	3,700	1,367	512	711
	3,500	1,369	512	710
	3,300	1,372	512	708
	3,000	1,376	512	706
	2,800	1,379	512	705
	2,600	1,382	512	703
p_b	2,344	1,386	512	701
	2,200	1,373	483	703
	1,900	1,348	424	707
	1,700	1,331	385	710
	1,500	1,314	346	714
	1,200	1,289	288	720
	1,000	1,272	249	725
	800	1,254	209	730
	500	1,223	146	742
	15	1,078	0	811

Step 2: Configure the value input and output units.

Step 3: Normalize total molar by entering components data (molar percent, molecular weight), reference data (reservoir temperature, reference depth/pressure).

Step 4: Enter specific gravity, choose the correlation method for boiling temperature, T_c, P_c, V_c, Omega. Also, compute the values of the pseudo components.

Step 5: Select the pure and pseudo component coefficients and compute the binary interaction coefficients.

Step 6: Choose a phase envelope test point, calculate the phase envelope, and plot the Phase diagram.

Step 7: Manual temperature and pressure range, and calculation CCE test.

Step 8: Manual range calculation (temperature and pressure), calculate DL test.

Step 9: Manual range calculation (temperature and pressure), calculate separator test.

Step 10: Enter lab data (P_{sat}, CCE, SEP, DL test).

Step 11: Setup for regression process by choosing mode, data and model

Option 3 is selected at Data Match Model: Individual OmegaA, OmegaB, and Pseudo T_{cs}, P_{cs}, AFs. Every component will have an eigenvalue of Omega A and B. Furthermore, the T_{cs}, P_{cs} and AF aggregated as well as the pseudo component will be provided for regression.

Step 12: Setup matching process - change OmegaA, OmegaB all components, change T_c, P_c, AF of pseudo components; change binary interaction coefficients of all pseudo components; and setup separator correction.

Step 13: Regression.

Step 14: Collect results and error details after regression.

Step 15: Repeat step 7 to step 9 to calculate the value of CCE, DL, separator test after matching process.

3.32. Simulation of fluid thermodynamic tests workflow

The initial phase of this procedure involves the input of essential parameters concerning both pure components and their corresponding pseudo components. Following this, under a specific set of pressure and temperature conditions, equilibrium ratios for individual components are approximated via correlations designed for real gasses. Subsequently, a flash calculation is executed, yielding critical information such as the compressibility factor and fugacity coefficient for both the liquid and gas phases. Leveraging this data, the equilibrium ratios are then precisely computed, capitalizing on the fugacity coefficient.

The process advances with a pivotal assessment of the convergence between the calculated equilibrium ratios and their assumed counterparts. If the convergence criteria are satisfied, the values for equilibrium ratios (K_i), liquid phase compositions (x_i), gas phase compositions (y_i), mole quantities for the liquid phase (n_L), mole quantities for the vapor phase (n_V), liquid phase compressibility factor (Z_L), and vapor phase compressibility factor (Z_V) are finalized as the solution. However, in instances where the convergence is not achieved, a new set of equilibrium ratios is assumed, based on the calculated equilibrium ratios from the prior iteration, and the entire calculation process is iteratively repeated until convergence is established.

This methodology, once successfully executed, paves the way for comprehensive simulations of fluid thermodynamic tests. Specifically, the application of the Peng-Robinson equation of state (EOS) is deployed to calculate critical component equivalent (CCE), differentially liberated (DL), and separator test parameters, spanning from Section 2.3.3 to 2.3.5.

3.4. Results & discussions

3.4.1. Regression results by PVTp software

The outcomes pertaining to relative volume, liquid density, gas - oil ratio, solution gas - oil ratio, and oil formation volume factor for the critical component equivalent (CCE), differentially liberated (DL), and separator tests are succinctly synthesized within Tables 7 - 13.

Within the framework of the critical component equivalent (CCE) examination, the relative volume undergoes evaluation across the pressure range from pi to pb. The empirical observations manifest an interval of relative volumes lying between 0.979 and 1. Meanwhile, the outcomes derived from the PVTp software exhibit a spectrum spanning from 0.975136 to 0.999939. An analysis of the data shows a cumulative disparity of 0.027189, encompassing the differential between the laboratory-derived measurements and the software-generated results.

The separator test is executed in two stages. In the initial stage, conducted at 158°F and 200 psia, the gas - oil ratio from laboratory data stands at 395 scf/bbl, while the corresponding output from the PVTp software gives a notably contrasting value of 358.005 scf/bbl. Furthermore,

Table 7. *Relative volume result at CCE test*

CCE test	Temp.	Pressure (psia)	Relative volume ($V_r = V_t/V_b$)		
			Measured value	Software value	Error
p_i	225.9	4,495	0.979	0.975136	0.003864
	225.9	4,300	0.981	0.977008	0.003992
	225.9	4,100	0.983	0.978993	0.004007
	225.9	3,900	0.985	0.981047	0.003953
	225.9	3,700	0.986	0.983174	0.002826
	225.9	3,500	0.988	0.985379	0.002621
	225.9	3,300	0.99	0.987667	0.002333
	225.9	3,000	0.993	0.991267	0.001733
	225.9	2,800	0.995	0.993788	0.001212
	225.9	2,600	0.997	0.996413	0.000587
p_b	225.9	2,344	1	0.999939	6.1E-05
Error					0.027189

Table 8. *Gas oil ratio result at separator test*

Separator test	Temperature (°F)	Pressure (psia)	GOR (scf/bbl)		
			Measured value	Software value	Error
Stage 1	158	200	395	358.005	36.995
Tank	60	15	46	36.4963	9.5037
Error					46.4987

Table 9. *Liquid density result at CCE test*

CCE test	Temperature	Pressure (psia)	Liquid density (kg/m^3)		
			Measured value	Software value	Error
p_i	225.9	4,495	716	758.775	42.775
	225.9	4,300	715	757.321	42.321
	225.9	4,100	714	755.786	41.786
	225.9	3,900	712	754.203	42.203
	225.9	3,700	711	752.572	41.572
	225.9	3,500	710	750.888	40.888
	225.9	3,300	708	749.148	41.148
	225.9	3,000	706	746.428	40.428
	225.9	2,800	705	744.534	39.534
	225.9	2,600	703	742.573	39.573
p_b	225.9	2,344	701	739.954	38.954
Error					451.182

Table 10. *Liquid density result at separator test*

Separator test	Temperature (°F)	Pressure (psia)	Liquid density (kg/m^3)		
			Measured value	Software value	Error
Stage 1	158	200	823	815.358	7,642
Tank	60	15	862	843.585	18,415
Error					26,057

Table 11. *Oil formation volume factor result at separator test*

Separator test	Temperature (°F)	Pressure (psia)	Oil FVF (B_o) (bbl/stb)		
			Measured value	Software value	Error
Stage 1	158	200	1.316	1.04432	0.27168
Tank	60	15	1	1	0
Error					0.27168

Table 12. *Oil formation volume factor result at DL test*

DL test	Temperature (°F)	Pressure (psia)	Oil FVF B_o (bbl/stb)		
			Measured value	Software value	Error
p_i	225.9	4,495	1.357	1.19734	0.15966
	225.9	4,300	1.359	1.19964	0.15936
	225.9	4,100	1.362	1.20208	0.15992
	225.9	3,900	1.364	1.2046	0.1594
	225.9	3,700	1.367	1.20721	0.15979
	225.9	3,500	1.369	1.20992	0.15908
	225.9	3,300	1.372	1.21273	0.15927
	225.9	3,000	1.376	1.21715	0.15885
	225.9	2,800	1.379	1.22024	0.15876
	225.9	2,600	1.382	1.22347	0.15853
p_b	225.9	2,344	1.386	1.2278	0.1582
	225.9	2,200	1.373	1.21714	0.15586
	225.9	1,900	1.348	1.19469	0.15331
	225.9	1,700	1.331	1.18017	0.15083
	225.9	1,500	1.314	1.16594	0.14806
	225.9	1,200	1.289	1.14493	0.14407
	225.9	1,000	1.272	1.13116	0.14084
	225.9	800	1.254	1.11737	0.13663
	225.9	500	1.223	1.09571	0.12729
	225.9	15	1.078	1.04504	0.03296
Error					2.94067

Table 13. *Liquid density result at DL test*

DL test	Temperature (°F)	Pressure (psia)	Calculated liquid density (kg/m^3)		
			Measured value	Software value	Error
p_i	225.9	4,495	716	758.775	42.775
	225.9	4,300	715	757.321	42.321
	225.9	4,100	714	755.786	41.786
	225.9	3,900	712	754.204	42.204
	225.9	3,700	711	752.572	41.572
	225.9	3,500	710	750.888	40.888
	225.9	3,300	708	749.148	41.148
	225.9	3,000	706	746.428	40.428
	225.9	2,800	705	744.534	39.534
	225.9	2,600	703	742.573	39.573
p_b	225.9	2,344	701	739.954	38.954
	225.9	2,200	703	743.351	40.351
	225.9	1,900	707	750.773	43.773
	225.9	1,700	710	755.741	45.741
	225.9	1,500	714	760.736	46.736
	225.9	1,200	720	768.322	48.322
	225.9	1,000	725	773.434	48.434
	225.9	800	730	778.636	48.636
	225.9	500	742	786.862	44.862
	225.9	15	811	818.17	7.17
Error					825.208

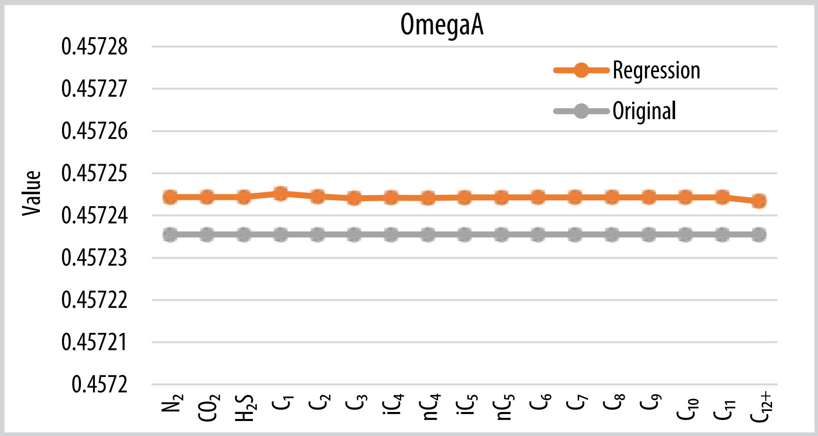

Figure 2. *Regressed OmegaA by PVTp software versus original data.*

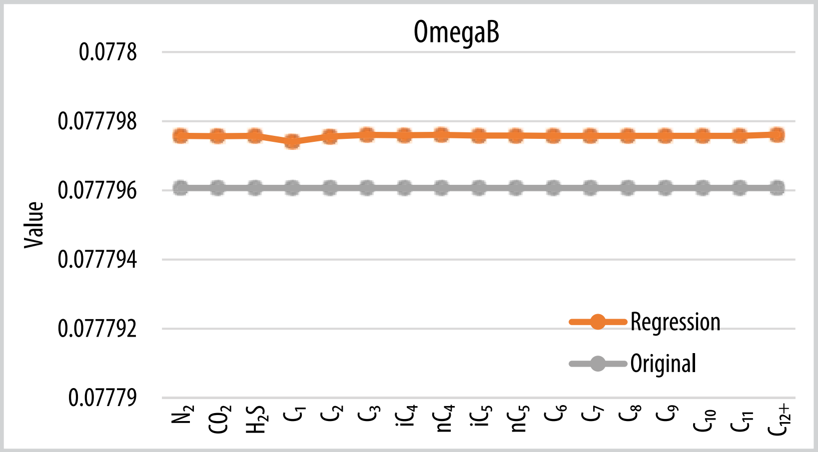

Figure 3. *Regressed OmegaB by PVTp software versus original data.*

during the subsequent stage under standard conditions, the gas - oil ratio is determined to be 46 scf/bbl based on laboratory findings, in stark contrast to the software-derived value of 36.4963 scf/bbl.

The liquid density values are ascertained across the pressure range from p_i to p_b. The experimental measurements indicate a range between 716 kg/m^3 and 701 kg/m^3, while the corresponding values generated by the PVTp software fall within the range of 758.775 kg/m^3 to 739.954 kg/m^3. It is noteworthy that there exists a substantial disparity of 451.182 between the laboratory data and the software results.

Liquid density from lab data is 823 kg/m^3 at stage 1 (158°F, 200 psia), contrasted to PVTp software result of 815.358 kg/m^3. Furthermore, the liquid density value from lab data and software findings at the standard condition stage is 862 kg/m^3 and 843.585 kg/m^3, respectively.

Oil FVF from lab data is 1.316 bbl/stb at stage 1 (158°F, 200 psia) compared to PVTp software result of 1.04432 bbl/stb. Furthermore, in the standard condition stage, the oil FVF value from lab data and software results are both equal to 1 bbl/stb.

In the DL test, the measured oil FVF increases from 1.357 bbl/stb at p_i to a peak of 1.386 bbl/stb at p_b. Then it decreases to 1.078 bbl/stb at 15 psia. Similarly, the software result rises from 1.19734 bbl/stb to 1.2278 bbl/stb, and drops to 1.078 bbl/stb.

The observed liquid density in the DL test drops from 716 kg/m^3 at p_i to 701 kg/m^3 at p_b, then climbs to 811 kg/m^3 at 15 psia. Similarly, the software result falls from 758.775 kg/m^3 to 739.954 kg/m^3 and then climbs to 818.17 kg/m^3.

- The comparison between original value of OmegaA, OmegaB by Peng-Robinson EOS and PVTp software regression process is shown in Figures 2 and 3.

The original OmegaA of P-R EOS is a constant value, 0.457235515; while the regressed one by software fluctuates between 0.457245171 and 0.457243413 with an average of 0.457244293.

The regressed OmegaB by software fluctuates between 0.077797614 and 0.0777974054 with an average of 0.077797572, while the original Omega A of P-R EOS is a constant value at 0.0777960718.

3.4.2. Simulation of fluid thermodynamic tests results

In Figure 4, the calculated value, software result, and measured data of the oil formation volume factor have roughly the same trend, increasing from p_i to reach a peak at p_b, then decreasing from p_b to 4,495 psia, although the measured data is always higher than two other types of values with an average gap of 0.15. Moreover, the calculated value and software result are relatively equal, except that at standard condition, the computed value is 0.964166283 bbl/stb, the software result is 1.04504 bbl/stb, and the observed data is 1.078 bbl/stb.

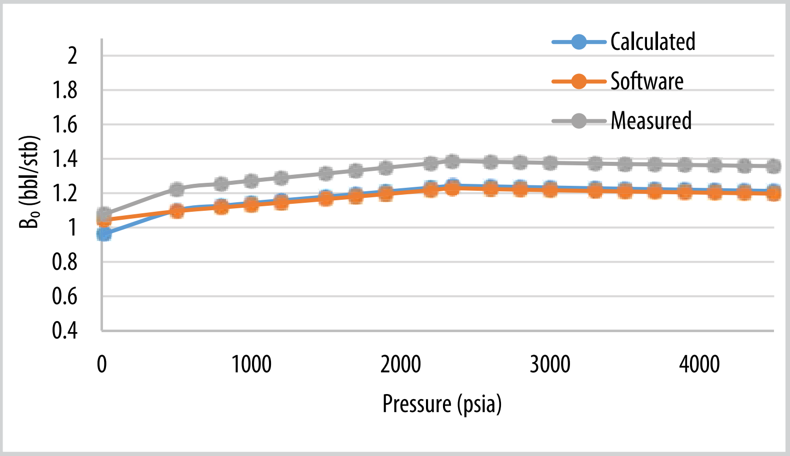

Figure 4. *Oil formation volume factor versus pressure.*

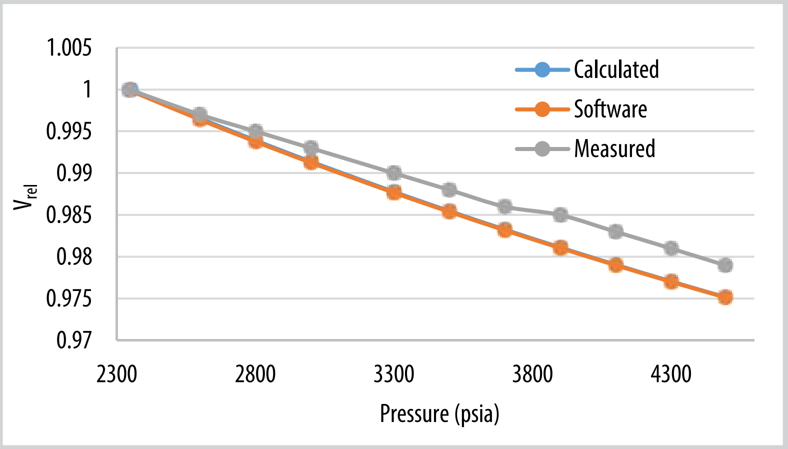

Figure 5. *Relative volume versus pressure.*

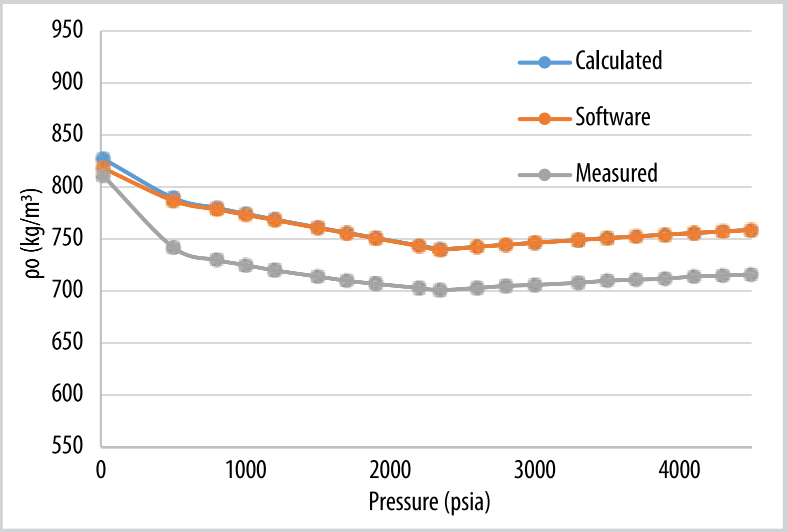

Figure 6. *Oil density versus pressure.*

In Figure 5, the value of relative volume is trending upward through the pressure range (from p_i to p_p). The calculated value and software result of relative volume are nearly the same at each spot of the measured pressure scheme. For measured data, the value at p_{sat} is roughly 1, similar to the calculated and software results. After that, measured data is always higher than two other kinds of values until the end. At 4,495 psia, the calculated value is 0.97518753, compared to 0.975136 at the software result and 0.979 at the measured data.

Figure shows that the calculated value, software result, and measured data of the oil formation volume factor have essentially the same pattern, falling from p_i to p_b, then rising from p_b to 4,495 psia, despite the fact that the measured data value is always smaller than the two others with an average gap of 45. Moreover, the calculated value and software result is significantly matched, except that at the standard circumstance, the calculated value is 827.2420778 kg/m^3, the software result is 818.17 kg/m^3, and the observed data is 811 kg/m^3.

4. Conclusion

In summary, this study has introduced a quantitative approach for simulating fluid thermodynamic tests, including CCE, DL, and separator tests, within multicomponent systems. This approach combines the utilization of equilibrium ratios, flash calculations, and the application of the Peng-Robinson equation of state. The calibration process, facilitated through the PVTp software regression procedure, allows the flexible determination of OmegaA and OmegaB values, thereby enhancing the precision of fluid thermodynamic test calculations and optimizing error margins in comparison to empirical data.

The efficacy of this proposed method has been substantiated through a set of numerical results. For instance, the bubble point pressure values extracted from observed data, software-generated values, and calculated outcomes stand at 2,344, 2,339, and 2,350.42 psia, respectively. In addition, the calculated results of various fluid thermodynamic tests, such as relative volume, oil formation volume factor, and liquid density, are close to those generated by the PVTp software and exhibit acceptable error levels compared to the measured data.

However, it is imperative to acknowledge that the DL test has revealed a substantial disparity in the solution gas - oil ratio. This incongruity emphasizes the necessity for more comprehensive measured data to enhance the simulation's accuracy and narrow the error gap.

The juxtaposition between the proposed methodology and the collected data underscores the suitability of integrating equilibrium ratios, flash calculations, and the Peng-Robinson equation of state as a dependable model for the precise calculation of equilibrium ratios and fluid thermodynamic tests within multicomponent systems. This approach provides a quantitative framework for simulating fluid thermodynamic tests, delivering valuable insights, and diminishing the dependence on costly laboratory experiments.

Acknowledgment

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