Development of a Computational Fluid Dynamics Compositional Wellbore Simulator for Modeling of Asphaltene Deposition

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ABSTRACT: The asphaltene problem is a two-step process: (1) asphaltene precipitation, as predicted by the thermodynamic model, and (2) asphaltene deposition, the amount of which is estimated by the kinetic model. Asphaltene precipitation is a prerequisite but not a sufficient condition for deposition. Deposition is dependent on other factors such as surface properties, phase behavior, rheology, and flow patterns. As a result, in addition to understanding thermodynamic and kinetic models, it is critical to also understand flow models. In fact, multiphase flow modeling is at the core of simulation, and it must be coupled with thermodynamic and kinetic models. Numerous studies on modeling asphaltene deposition on pipe walls have been performed theoretically and experimentally, but a comprehensive theory to properly understand this phenomenon has not yet been presented. In thermodynamic modeling, the perturbed chain statistical associating fluid theory (PC-SAFT) equation of state is used to predict the asphaltene phase behavior. In this study, we show that the proposed PC-SAFT model is more accurate than the solid model used in commercial software. Unlike prior research that neglected flow patterns or used empirical relations to model multiphase flow, this study simulates multiphase flow using separate momentum equations for each phase. Among the existing kinetic models, the Kurup model has been used to predict the asphaltene deposition profile in the wellbore due to its greater compatibility for computational fluid dynamics application. The results of the proposed model show good agreement with field case data of asphaltene deposition thicknesses along the wellbore tubing.

1. INTRODUCTION

During oil production, multiphase flow usually occurs in different parts of a flow line such as wells, pipes, and surface equipment. The destructive effect of various flow assurance issues and flow disturbance with solid particle deposition has also added to the challenge of wellbore modeling in simulators. Predicting how much asphaltene will be deposited in the wellbore at any given time and place will allow the industry to adopt an appropriate strategy to increase the efficiency of the operation process and to avoid the risks associated with asphaltene deposition.

Modeling of asphaltene deposition in the wellbore can be divided into three parts: (1) thermodynamic modeling of asphaltene precipitation, (2) multiphase flow modeling in the wellbore, and (3) modeling the deposition of asphaltene particles on the surface.

Thermodynamic prediction models of asphaltene deposition mentioned in various sources and papers can be classified into six groups.1 These models are solubility models,2 colloidal models,3 micellization models,4,5 solid models,6 Cubic-Plus-Association (CPA) model,7 and perturbed chain statistical associating fluid theory (PC-SAFT) model.8–11 In this research, the PC-SAFT state equation is used to simulate the phase behavior of asphaltene. Because it takes into account the interaction of molecules, the PC-SAFT state equation gives a more accurate result for modeling the asphaltene phase behavior.9

Several analytical and numerical methods for modeling multiphase flows in wellbores have been proposed in recent years. Empirical correlations have been proposed by Dukler et al.,12,13 Hagedorn and Brown,14 Beggs and Brill,15 and Mukherjee and Brill16 based on laboratory data in a specific range of oil and gas velocities. Another approach for simulating multiphase flow is to use conservation, momentum, and energy equations. Yuan and Zhou17 compared models based on empirical correlations and models based on transport equations and concluded that equations based on empirical correlations...
Table 1. PC-SAFT Parameters of Correlations for Heavy Gas, Saturates, Aromatics + Resins, and Asphaltene

| Component     | H₂S  | N₂    | CO₂  | Methane | Heavy gas | Saturates | Aromatics + resins | Asphaltene |
|---------------|------|-------|------|---------|-----------|-----------|-------------------|------------|
| H₂S           | 0    |       |      |         |           |           |                   |            |
| N₂            | 0.09 |       |      |         |           |           |                   |            |
| CO₂           | 0.0678 | 0 | 0 |         |           |           |                   |            |
| Methane       | 0.062 | 0.03  | 0.05 | 0       |           |           |                   |            |
| Heavy gas     | 0.07 | 0.075 | 0.12 | 0.03    | 0         |           |                   |            |
| Saturates     | 0.09 | 0.14  | 0.13 | 0.03    | 0.005     | 0         |                   |            |
| Aromatics + resins | 0.015 | 0.158 | 0.10 | 0.029  | 0.012 | 0.007 | 0 |            |
| Asphaltene    | 0.015 | 0.158 | 0.10 | 0.029  | 0.012 | 0.007 | 0 |            |

are only applicable in a limited range of velocities, while models based on transport equations provide acceptable results in a broad range of liquid and gas velocities.

Models based on transport equations are classified into two types. The first group, known as the homogeneous model, ignores slippage between phases and assumes that all fluids move at the same velocity.¹⁹ The assumption of nonslip in multiphase flow is invalid due to the difference in viscosity and density between the phases. Two approaches are included in the second group, which recognize slippage between phases. The first approach is drift flux presented by Kaichiro and Ishii,¹⁹ and the second method is the two-fluid model presented by Taitel and Dukler.²⁰ Slippage between phases is considered in the drift flux model by a correlation that relates the velocity of the fluid mixture to the velocities of oil and gas. Due to the fact that the drift flux model assumes slippage between phases, it misrepresents the momentum of the transition between phases for separated flow patterns such as annular flow. Instead of considering the slip velocity by empirical correlations, separate momentum equations are used for each phase in two-fluid models. The interaction of forces between phases, as well as between fluids and walls, is described in each phase’s momentum equation using this method. Some researchers, such as Stone,²¹ Winterfeld,²² and Pourafshary,²³ have used the two-fluid model to simulate multiphase flow. Other researchers, such as Hasan and Kabir²⁴,²⁵ and Livescu et al.²⁶ have used the drift flux model.

Because of a lack of knowledge of the physics governing asphaltene deposition, its modeling is highly dependent on experimental data. In the work of Souljani et al.,²⁷ the asphaltene deposition rate is fitted to a simple equation with the exponential Arrhenius function for temperature. In this equation, it is assumed that asphaltene precipitation is controlled by the mechanism of a chemical reaction. Shirdel et al.²⁸ compared the predictions of different mechanistic deposition models on the existing experimental data. The concept of particle–wall collision efficiency was investigated by Eskin et al.²⁹ and Akbarzadeh et al.³⁰ In their models, it is assumed that relatively large particles do not deposit on the wall and smaller particles generally do not deposit at a single collision (the probability of particle deposition is very low). Vargas et al.³¹ and Kurup et al.³² considered asphaltene deposition as a first-order kinetics. Their model appears to be very appropriate for computational fluid dynamics (CFD) application.

In this research, we improve the PC-SAFT model to more accurately predict asphaltene precipitation and also compare the proposed model with the solid model of CMG WinProp software. Due to the complexities of solving multiphase equations and coupling the thermodynamics and kinetics of asphaltene with fluid flow dynamics, most asphaltene deposition models place more emphasis on kinetics and thermodynamics and do not consider multiphase fluid flow patterns. In this study, we used powerful CFD tools to model multiphase flow. The Kurup model is used among the available kinetic models to predict the wellbore asphaltene deposition profile, which is more compatible with CFD due to derivation based on transport equations.

2. THERMODYNAMIC MODELING MODULE

According to the earlier study of PC-SAFTs, a composition of H₂S, N₂, CO₂, C1, and four pseudocomponents is converted into a recombinated crude oil: heavy gas, saturates, aromatics + resins, and asphaltenes. The details of the characterization methodology in the PC-SAFT model for predicting asphaltene precipitation are presented in previous works.³³–³⁵ PC-SAFT EOS parameters for H₂S, N₂, CO₂, and CH₄ are available in the literature.⁰ There are correlations for the other components as shown in Table 1.²⁴ The PC-SAFT parameters for aromatics and resins depend on the molecular weight and aromaticity value for aromatics + resins. The molecular weight value is determined in the characterization, but the aromaticity value is obtained from the optimization process. The PC-SAFT parameter for asphaltene depends on the aromaticity value for asphaltene and the molecular weight, both of which are obtained from optimization.

According to previous research, the aromaticity value for aromatics + resins, as well as the aromaticity value and molecular weight for asphaltene, was adjusted separately to match experimental data, without taking into account the simultaneous effect of the parameters on bubble pressure and asphaltene experimental data.³⁵–³⁶ Moreover, the experimental data on asphaltene precipitation have not been matched in previous
The parameters related to PC-SAFT for aromatics + resins and asphaltene are estimated in this work by simultaneously fitting the predicted bubble pressure, density, asphaltene onset pressure, and amount of asphaltene precipitation to experimental data. Unlike previous studies, which did not provide a general rule for binary interaction parameters between asphaltene and other components, in this study, we provided a constant set of binary interaction parameters, and if the agreement with experimental data is not good, one or two of the binary interaction parameters between asphaltene and other components were placed as adjustment parameters in the optimization process. The constant set of binary interaction parameters can be seen in Table 2.

2.1. Flash Calculation. Because the number of equilibrium phases is unknown before performing multiphase flash calculations, its complexity increases. The precipitated asphaltene is considered to be a liquid phase and is modeled using PC-SAFT EOS at liquid/liquid equilibrium or vapor/liquid/liquid equilibrium. In this simulator, we used a robust algorithm for performing multiphase flash calculations. The calculation procedure is shown in Figure 1.

$$K_i = \frac{y_i}{x_i}$$

The following equations are used for the calculation of oil and gas phase compositions:

$$x_{i,1} = \frac{z_i}{1 + n_v(K_{i,1} - 1) + n_{l2}(K_{i,2} - 1)}$$

$$y_{ig} = K_{i,1} x_{i,1}$$

$$x_{i,2} = K_{i,2} x_{i,1}$$

Independent unknowns for thermodynamic modeling of asphaltene are $K_{i,1}, K_{i,2}, n_v$, and $n_{l2}$, which gives $2n_v + 2$ independent variables. We presented the same number of equations above. Quasi-Newton successive substitution (QNSS), which does not require a good initial guess, is used to solve these equations. The algorithm used in the simulator to perform liquid/liquid/vapor flash is described in detail in Figure 2.

2.2. Validation of the Thermodynamic Model. We use experimental data from one of the Iranian oil fields to validate the proposed thermodynamic model. The properties of crude oil are summarized in Table 3. The composition of crude oil is provided in Table 4. The saturation pressure and upper and lower onset pressures are given in Table 5. Table 6 shows the precipitation data. Table 7 lists the results of the characterization using PC-SAFT methods. Figure 3 shows the results of three simulations with different binary interaction parameters. The first case without considering the binary interaction parameters between asphaltene and other components as optimization parameters, the second case with considering only binary interaction parameters of asphaltene with saturates and methane as optimization parameters, and the third case with considering binary interaction parameters between all components and asphaltene as optimization parameters are included for these three runs. As can be seen, in the first case, there is a large difference with the experimental data, especially in lower onset pressure, bubble pressure, and the amount of asphaltene precipitation. In relation to upper onset pressure, all three runs have good predictions, although the predictions of the first case are more accurate. The second and third cases predict the value of lower onset pressure more accurately, and the first case shows the value of lower onset pressure twice as much as the
experimental value. This figure shows that not considering the binary interaction parameters between asphaltene and other components as optimization parameters may not be in good agreement with the experimental data. Also, to achieve a good match, we do not need to consider the binary interaction parameters of all components with asphaltene as adjustment parameters. Considering the binary interaction parameters of asphaltene with saturates and methane is sufficient to have a good agreement with experimental data.

2.2.1. Comparison of the Proposed PC-SAFT Model with the Solid Model.

Table 3. Fluid and Reservoir Properties of One of Iran’s Oil Fields

| parameters                  | value  |
|------------------------------|--------|
| reservoir temperature (°F)   | 185    |
| reservoir pressure (psia)    | 3380   |
| GOR (SCF/STB)                | 598    |
| API gravity (deg)            | 24     |
| SARA analysis (%, w/w)       |        |
| saturates                    | 65.46  |
| aromatics                    | 19.44  |
| resins                       | 6.4    |
| asphaltene                   | 8.7    |

Table 4. Modeled Fluid Composition for One of Iran’s Oil Fields

| component   | flashed liquid (mol %) | flashed gas (mol %) | reservoir fluid (mol %) |
|-------------|------------------------|---------------------|-------------------------|
| H2S         | 0.00                   | 1.00                | 0.59                    |
| N2          | 0.00                   | 0.10                | 0.06                    |
| CO2         | 0.00                   | 4.13                | 2.45                    |
| C1          | 0.00                   | 65.18               | 38.65                   |
| C2          | 0.19                   | 11.10               | 6.66                    |
| C3          | 1.05                   | 8.26                | 5.33                    |
| i-C4        | 0.40                   | 1.43                | 1.01                    |
| n-C4        | 1.50                   | 3.90                | 2.92                    |
| i-C5        | 1.29                   | 1.20                | 1.24                    |
| n-C5        | 1.73                   | 1.35                | 1.51                    |
| C6          | 9.63                   | 1.27                | 4.67                    |
| C7          | 10.11                  | 0.75                | 4.56                    |
| C8          | 8.80                   | 0.29                | 3.75                    |
| C9          | 5.44                   | 0.04                | 2.24                    |
| C10         | 6.26                   | 0.00                | 2.55                    |
| C11         | 5.55                   | 0.00                | 2.26                    |
| C12         | 48.05                  | 0.00                | 19.56                   |
| total       | 100.00                 | 100.00              | 100.00                  |
| Mw (g/mol)  | 290                    | 25.82               | 111                     |
| C12 + Mw (g/mol) | 492          |
| C12 + density (g/cm³) | 0.9569 |

Table 5. Saturation Pressure and Asphaltene Onset Pressures from Experimental Data for One of Iran’s Oil Fields

| temperature (°F) | saturation pressure (psia) | upper onset pressure (psia) | lower onset pressure (psia) |
|------------------|----------------------------|-----------------------------|-----------------------------|
| 185              | 2747                       | 5002                        | 564                         |

Table 6. Precipitated Asphaltene Experimental Data for One of Iran’s Oil Fields

| pressure (psia) | precipitated asphaltene (wt %) |
|-----------------|--------------------------------|
| 3418            | 1.03                           |
| 3218            | 1.16                           |
| 2918            | 1.25                           |
| 2216            | 0.94                           |
| 1015            | 0.34                           |

Table 7. PC-SAFT Parameters for One of Iran’s Oil Fields

| component       | Mw (g/mol) | composition (mol %) | m | σ (Å) | ε/k (K) |
|-----------------|------------|---------------------|---|------|--------|
| H2S             | 34.08      | 5.3                 | 1.65 | 3.073 | 227.34 |
| N2              | 28.01      | 0.057               | 1.205 | 3.313 | 90.96  |
| CO2             | 44.01      | 2.3                 | 2.073 | 2.785 | 169.21 |
| methane         | 16.04      | 38.41               | 1.000 | 3.704 | 150.03 |
| heavy gas       | 45.70      | 16.56               | 2.08  | 3.62  | 205.8  |
| saturates       | 247.95     | 31.9                | 7.22  | 3.94  | 254.3  |
| aromatics + resins (γ = 0.525) | 324.13 | 9.63 | 6.42  | 4.18 | 381.2 |
| asphaltene (γ = 0.466) | 833.9 | 0.62 | 1.65 | 4.28 | 385.8 |

parameters of all components with asphaltene as adjustment parameters. Considering the binary interaction parameters of asphaltene with saturates and methane is sufficient to have a good agreement with experimental data.

2.2.1. Comparison of the Proposed PC-SAFT Model with the Solid Model. Solid models are the most common models of
asphaltene precipitation simulations in commercial software. In this section, we compare the PC-SAFT model presented with the solid model of CMG WinProp software. In Figure 4, we show the simulation results of three cases. The first case is related to the proposed PC-SAFT model without considering binary interaction parameters between asphaltene and other components as optimization parameters. The second case shows the results of asphaltene precipitation simulation based on the PC-SAFT model and considering binary interaction parameters between asphaltene with methane and saturates as optimization parameters. The third case shows the simulation results obtained from CMG WinProp software. As can be seen, among the simulation results, the highest agreement with the experimental data of precipitation and asphaltene onset pressures is related to the second case. Only the bubble pressure obtained from CMG WinProp is slightly better than the second case. The main problem with the CMG WinProp simulation results is the huge difference between upper onset pressure and lower onset pressure modeled with experimental data. There is a difference of about 800 psia between the experimental data of asphaltene onset pressures and the CMG WinProp simulation results. The key reason for this problem is that asphaltene onset pressure data was not taken into account during the optimization process.

The results of the PC-SAFT model can be seen in Figure 5 if, like the solid model, the asphaltene onset pressure data are not considered in the optimization. Also, in this run, only three parameters, the aromaticity value for aromatics + resins and aromaticity value and molecular weight for the asphaltene, are set as adjustment parameters, and binary interaction parameters do not change. In this case, the bubble pressure and amount of asphaltene precipitation are relatively in agreement with the experimental data, but predicting the upper and lower onset pressures is extremely inaccurate. As shown in Figure 5, the solid model error is less than this case.

3. MULTIPHASE FLOW MODEL
As previously stated, asphaltene deposition simulation is divided into three parts, the most important of which is multiphase flow simulation. To simulate multiphase flow, the simulator must solve four equations to obtain the four primary variables. The four primary variables are liquid volume fraction ($\alpha_1$), pressure $P$, and velocities $U_{li}$. The Schematic view of staggered gridding arrangement is shown in Figure 6.
(P), gas velocity \( (u_g) \), and liquid velocity \( (u_l) \). To solve these variables, the same number of equations is required. With these assumptions, we tried to model multiphase flow: (1) one-dimensional flow. (2) The liquid phase will include the oil and asphaltene-rich phase. The asphaltene-rich phase is defined as a liquid phase whose components will be exactly the components of crude oil, except that the asphaltene component is considered in precipitated form. Oil and asphaltene-rich phases have the same velocities. (3) Both gas and liquid have the same temperature and pressure. (4) We use the concept of staggered grid to discretize the transport equations. In a staggered grid arrangement, scalar variables such as pressure and hold-up are calculated in the control volume center, while the phase velocities are calculated in cell faces, as shown in Figure 6. Mass conservation and momentum conservation equations are fundamental equations in the simulation of multiphase flows.

\[
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) = \frac{\partial}{\partial x}(\rho u) + \rho g \sin \theta - \alpha_i R_{dep} \tag{10}
\]

\[
\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) = -\alpha_i \frac{\partial P}{\partial x} + \rho u \frac{\partial u}{\partial x} + \rho g \sin \theta - K \frac{\rho_{avg}}{D} \frac{\partial u}{\partial x} + F_D \tag{11}
\]

The shear stress of the turbulent flow is modeled in momentum equations by a wall friction force. For dispersed fluid, the value \( K = 0 \), and for continuous fluid, the value \( K = 1 \).

The shear stress between the phases is displayed as drag force and with the variable \( F_D \) in the momentum equations. This force is highly dependent on the flow regime and is summarized in Table 8.

3.1. Discretization Form of the Momentum Equation.

\[
\frac{(\alpha_i \rho_{avg})^n (u_i)^{n+1} - (\alpha_i \rho_i u_i)^n}{\Delta t} + \frac{(\alpha_i \rho_{avg})^n(u_i)^{n+1}}{z_{is} - z_{is+1}} = \frac{-\alpha_i \rho_{avg}^n \frac{\partial u_i}{\partial x}}{z_{is} - z_{is+1}} - \frac{\alpha_i \rho_{avg}^n \frac{\partial u_i}{\partial x}}{z_{is} - z_{is+1}} + 144 \rho \frac{P_{avg}}{z_{is} - z_{is+1}} + \frac{(\alpha_i \rho_{avg})^n}{z_{is} - z_{is+1}} - f_{avg} \Delta t \tag{12}
\]
Table 8. Drag Force Calculation for Different Flow Regimes

\[ d_b = 3.28 \left( \frac{6 \times 10^{-11}(1 - \alpha_i)}{\pi} \right)^{1/3} \]

\[ N_{hub} = 1488.16 \left( \frac{\rho_l u_g - \rho_g u_b}{\mu_l} \right) \]

bubbly flow

\[ CD = 24 \left( \frac{1 + 0.15N_{hub}^{0.67}}{N_{hub}} \right) N_{hub} \leq 1000 \]

\[ CD = 0.44N_{hub} > 1000 \]

\[ CD_{1g} = CD \times \alpha_i^{0.37} \]

\[ F_{lag} = 0.75CD_{1g}(1 - \alpha_i)\alpha_i'\rho_l(u_g - u_l) \]

\[ u_l = 0.48\alpha_i^{0.37} = 0.3 \]

\[ u_g = \left(1 - \alpha_i\right) - \left(1 - \alpha_i^{0.37}\right) \]

\[ a_{slug} = 3.6(1 - \alpha^{0.37}) \]

\[ F_{lag} = \frac{0.01\sqrt{(1 - \alpha_i)(1 + 75\alpha_i)\rho_l(u_g - u_l)}}{D} \]

\[ a_{slug} = 3.6(1 - \alpha^{0.37}) \]

\[ F_{lag} = \frac{0.01\sqrt{(1 - \alpha_i)(1 + 75\alpha_i)\rho_l(u_g - u_l)}}{D} \]

slug flow

\[ P = P^* + P' \]

If we replace the correct pressure in the momentum equations (eqs 17 and 18), it leads to the calculation of the correct liquid velocity and the correct gas velocity, and if we substitute the assumed pressure in eqs 17 and 18, we get the following equations:

\[ (a_{i-n} - a_{i})_{i} \langle u_{i} \rangle_{i} + \langle a_{i} \rangle_{i} \langle u_{i} \rangle_{i} \]

\[ = a_{i-n+1,1}(u_{i})_{i} + a_{i-n+1,1}(u_{i})_{i} + a_{i-n,1}(P_{i} - P_{i+1}) + (b_{i})_{i} \]

\[ (a_{i-n} - a_{i})_{i} \langle u_{i} \rangle_{i} + \langle a_{i} \rangle_{i} \langle u_{i} \rangle_{i} \]

\[ = a_{i-n+1,1}(u_{i})_{i} + a_{i-n+1,1}(u_{i})_{i} + a_{i-n,1}(P_{i} - P_{i+1}) + (b_{i})_{i} \]

T o s o l v e f o u r d y n a m i c v a r i a b l e s

\[ p_{i}^{*+1}, u_{i}^{*+1}, u_{g}^{*+1}, \text{and} \ a_{i}^{*+1}, \text{four initial assumptions} \]

\[ p_{i}^{*}, u_{i}^{*}, u_{g}^{*}, \text{and} \ a_{i}^{*} \text{are made. For this purpose, eqs 17 and} \]

\[ u_{i}, u_{i}^{*}, \text{and} \ u_{g}^{*}, \text{are defined as the correct liquid velocity, the correct gas velocity, and the correct pressure, and} \]

\[ u_{i}, u_{i}^{*}, \text{and} \ P \text{are defined as correction variables,} \]

\[ u_{i} = u_{i}^{*} + u'_{i} \]

\[ u_{g} = u_{g}^{*} + u'_{g} \]
\[
\begin{align*}
(a_{11,iv} - (a_{21})_{iv})(u_g - u_g^*)_{iv} + (a_{21})_{iv}(u_i - u_i^*)_{iv} \\
= a_{11,iv-1}(u_g - u_g^*)_{iv-1} + a_{11,iv+1}(u_g - u_g^*)_{iv+1} + a_{iv,pg} \\
\left((P_i - P_{oi}) - (P_{oi+1} - P_{oi+1}^{ii})\right)
\end{align*}
\]

(33)

According to eqs 27–2829

\[
\begin{align*}
(a_{11,iv} - (a_{21})_{iv})(u_i'_{iv}) + (a_{21})_{iv}(u_{g'}_{iv}) \\
= a_{11,iv-1}(u_i'_{iv-1}) + a_{11,iv+1}(u_i'_{iv+1}) + a_{iv,pg} \\
(P_i - P_{oi+1})
\end{align*}
\]

(34)

\[
\begin{align*}
(a_{11,iv} - (a_{21})_{iv})(u_g'_{iv}) + (a_{21})_{iv}(u_i'_{iv}) \\
= a_{11,iv-1}(u_g'_{iv-1}) + a_{11,iv+1}(u_g'_{iv+1}) + a_{iv,pg} \\
(P_i - P_{oi+1})
\end{align*}
\]

(35)

Assuming equivalent velocity corrections in neighboring control volumes,

\[
\begin{align*}
(u_i'_{iv}) & \approx (u_i'_{iv-1}) \approx (u_i'_{iv+1}) \\
(u_i'_{iv}) & = \frac{a_{iv,pg}}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}(P_i - P_{oi+1}) \\
& \quad + \frac{(a_{v,pg})}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}(u_i'_{iv}) \\
(u_g'_{iv}) & = \frac{a_{iv,pg}}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}(P_i - P_{oi+1}) \\
& \quad + \frac{(a_{v,pg})}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}(u_i'_{iv})
\end{align*}
\]

(36)

(37)

\[
\begin{align*}
G_{iv,pg} & = \frac{a_{iv,pg}}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}G_{iv,Dlg} \\
& = \frac{(a_{v,pg})}{a_{iv,pg} + a_{11,iv-1} + a_{11,iv+1}}
\end{align*}
\]

(38)

(39)

Divide eqs 37 and 38 by \(P_i - P_{oi+1}\),

\[
\begin{align*}
\frac{(u_i'_{iv})}{P_i - P_{oi+1}} & = \frac{(u_i'_{iv})}{P_i - P_{oi+1}}(u_i'_{iv}) \\
(\lambda_i'_{iv}) = G_{iv,pg} + G_{iv,Dlg}(\lambda_i'_{iv} - \lambda_i'_{iv}) \\
(\lambda_i'_{iv}) = G_{iv,pg} + G_{iv,Dlg}(\lambda_i'_{iv} - \lambda_i'_{iv}) \\
\left\{(1 - G_{iv,Dlg})\lambda_i'_{iv} + G_{iv,Dlg} \lambda_i'_{iv} = G_{iv,pg}
\right\}
\end{align*}
\]

(40)

(41)

(42)

(43)

(44)

\[
\lambda_i'_{iv} = \frac{G_{iv,pg}}{1 - G_{iv,Dlg}} - \frac{G_{iv,pg}}{1 - G_{iv,Dlg}} \lambda_i'_{iv} = \frac{G_{iv,pg}}{1 - G_{iv,Dlg}} - \frac{G_{iv,pg}}{1 - G_{iv,Dlg}}
\]

According to eqs 27–2829,

\[
\begin{align*}
(u_i)_{iv} & = (u_i^*)_{iv} + (\lambda_i'_{iv})(P_i - P_{oi+1}) \\
(u_i)_{iv} & = (u_i^*)_{iv} + (\lambda_i'_{iv})(P_i - P_{oi+1})
\end{align*}
\]

(45)

(46)

(47)

(48)

To calculate \(P_i\) to correct the velocity and pressure field, we substitute \(u_i\) and \(u_g\) in the overall continuity equation,

\[
\begin{align*}
(a_{iv,pg})(u_i)_{iv} - a_{iv-1,pg}(u_i)_{iv-1} + a_{iv,pg}(u_i)_{iv} - a_{iv-1,pg}(u_i)_{iv-1} \\
= b_{iv,pg} + b_{iv,pg}
\end{align*}
\]

(49)

\[
\begin{align*}
(a_{iv,pg}) = \frac{(a_{iv,pg})^*}{G_{iv,pg}} = \frac{(a_{iv,pg})^*}{G_{iv,pg}} + \frac{(a_{iv,pg})^*}{G_{iv,pg}}
\end{align*}
\]

(50)

(51)

(52)

(53)

\[
\begin{align*}
(a_{iv,pg})(u_i)_{iv} + (\lambda_i'_{iv})(P_i - P_{oi+1}) - a_{iv-1,pg} \\
((u_i^*)_{iv-1} + (\lambda_i'_{iv-1})(P_i - P_{oi+1}) \\
+ a_{iv,pg}(u_i^*)_{iv} + (\lambda_i'_{iv})(P_i - P_{oi+1}) \\
- a_{iv-1,pg}(u_i^*)_{iv-1} + (\lambda_i'_{iv-1})(P_i - P_{oi+1})) \\
= b_{iv,pg} + b_{iv,pg}
\end{align*}
\]

(54)

(55)

(56)

(57)

(58)

\(P_i\) is obtained by solving eq 54, and convergence occurs when \(b^*\); becomes zero. If \(b^*\) is not zero, the velocity and pressure fields

must be corrected by eqs 46–48.
After solving the velocity and pressure equations, the hold-up equation must be solved,
\[
a_{t;s}a_i(a_i)_{ls} + a_{t-1,s}a_i(a_i)_{ls-1} = b_{t;s}
\]  
(59)
\[
a_{t;s}a_i = \frac{(\rho_{a_i})_{ls}^n}{\Delta t} + \left(\frac{\alpha_{ls}^n}{(\rho_{a_i})_{ls}^n}\right)_{lv} + (K_{pre})_{ls}(C_{pre})_{ls}^n
\]  
(60)
\[
a_{t-1,s}a_i = -\frac{(\alpha_{ls}^n)_{lv}(\rho_{a_i})_{ls-1}^n}{z_{lv} - z_{lv+1}}
\]  
(61)
\[
b_{t;s}a_i = \frac{(\alpha_{ls}^n)_{lv}}{\Delta t} + \left(\Gamma^{int}\right)_{ls}
\]  
(62)

4. DEPOSITION KINETIC MODEL

Based on the kinetic models proposed by Vargas et al., Kurup et al., and Guan et al., two other important equations are added to the set of equations, which are the mass conservation of asphaltene in the dissolved state \((C_{dis})\) and in the precipitated state \((C_{pre})\),
\[
\frac{\partial (a_i C_{dis})}{\partial t} + \frac{\partial (a_i u_i C_{dis})}{\partial x} = -a_i R_{pre}
\]  
(63)
\[
\frac{\partial (a_i C_{pre})}{\partial t} + \frac{\partial (a_i u_i C_{pre})}{\partial x} = a_i R_{pre} - a_i R_{agg} - a_i R_{dep}
\]  
(64)
\[
R_{pre} = \begin{cases} K_{pre} (C_{dis} - C_{eq}) & C_{dis} \geq C_{eq} \\ -k_{dis} C_{pre} & C_{dis} < C_{eq} \end{cases}
\]  
(65)
\[
R_{agg} = K_{agg} C_{pre}
\]  
(66)
\[
R_{dep} = K_{dep} C_{pre}
\]  
(67)
\(C_{dis}\) is the concentration of dissolved asphaltene in the liquid phase at the thermodynamic equilibrium, calculated by PC-SAFT. \(C_{dis}\) is the actual concentration of dissolved asphaltene in the liquid phase. \(C_{pre}\) is the concentration of precipitated asphaltene in the liquid phase. \(R_{pre}\), \(R_{agg}\) and \(R_{dep}\) are the rate of asphaltene precipitation, asphaltene aggregation, and asphaltene deposition, respectively.

5. RESULTS AND DISCUSSION

In this section, we will verify the proposed model. The basis of the simulation verification is based on the data reported from the Kuwait Marrat field published by Kabir et al. Fluid and well properties for the Kuwait’s Marrat oil field are listed in Table 9. The composition of crude oil is given in Table 10. Experimental data of upper onset pressure and bubble pressure can be seen in Table 11. PC-SAFT parameters of this case are summarized in Table 12. Figure 8 depicts the asphaltene phase envelope after constructing the thermodynamic model and determining all of the parameters of the PC-SAFT equation of state. Although there are no experimental data on the amount of asphaltene deposition in the literature, due to the wide temperature range encountered in the wellbore and the importance of not failing the thermodynamic model at different temperatures, Figure 9 depicts the amount of asphaltene precipitation in terms of pressure at three temperatures: 120, 180, and 240 °F.
The operating conditions reported for wellhead are 320 psia and 120 °F. For the bottom hole, a pressure of 8500 psia and a temperature of 230 °F were reported. Multiphase simulation is performed by combining thermodynamic, dynamic, and kinetic modules to obtain the amount of asphaltene deposition in the wellbore. The algorithm used to achieve this goal is shown in Figure 7. Table 13 lists the kinetic coefficients reported in the study by Guan et al. for the Marrat oil field. All of the reported results are after 60 days from the start of production. Gas and liquid velocity profiles along the well are shown in Figure 10. As can be seen, the maximum asphaltene deposition occurs at a depth of 2200 ft to the wellhead, we will see only two phases of oil and gas and there will be no sign of asphaltene deposition. As can be seen, the maximum asphaltene deposition occurs at a depth of
4900 ft. Figure 12 confirms the results of Figure 10, and maximum deposition occurs in the same depth range.

A sensitivity analysis on the flow rate, which actually shows the effect of the Reynolds number on the asphaltene deposition profile, was performed for three different cases. As shown in Figure 13, asphaltene deposition decreases as the flow rate increases. The area below the graph shows the total mass of the deposited asphaltene. As can be seen, the area below the graph decreases with the increasing flow rate. Another point that is obvious in this figure is the displacement of the maximum thickness of asphaltene deposition due to the change in the flow rate. As the flow rate increases, the maximum deposit thickness is located closer to the wellhead.

6. CONCLUSIONS

In this work, the PC-SAFT model is used to model asphaltene precipitation. We propose three major modifications to improve the thermodynamic modeling of asphaltene precipitation compared to previous studies. First, the aromaticity value for aromatics + resins and aromaticity value and molecular weight for the asphaltene must be optimized simultaneously. Second, a constant set of binary interaction parameters was presented, and if the agreement with experimental data was poor, one or two of the binary interaction parameters between asphaltene and other components were placed as adjustment parameters in the optimization process. Third, not only bubble pressures, asphaltene onset pressures, and density experimental data but also asphaltene precipitation data are involved in the optimization process. When the proposed PC-SAFT model and CMG WinProp results are compared with experimental data, the PC-SAFT model predicts the asphaltene phase behavior more accurately. To develop a hydrodynamic simulator of asphaltene deposition, a thermodynamic simulator of asphaltene precipitation is combined with a multiphase flow simulator in which the continuity, momentum, and asphaltene deposition kinetic equations are solved simultaneously. We used the powerful CFD tool to simulate multiphase flow. Also, to model the kinetics of asphaltene deposition, among the various models that are available, the model of Kurup et al., which is more compatible with CFD, was used. Finally, the results of the proposed model were compared with field case data of the asphaltene deposition thickness along the wellbore tubing.

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NOMENCLATURE

\(K_i\) = equilibrium ratio (K value) of component \(i\)  
\(x\) = liquid composition  
\(y\) = vapor composition  
\(z\) = overall composition  
\(n_v\) = vapor mole fraction  
\(n_{12}\) = asphaltene-rich phase mole fraction  
\(q_i\) = fugacity coefficient of component \(i\)  
PC-SAFT = perturbed-chain statistical associating fluid theory  
\(a_i\) = hold-up of phase \(j\) (\(j = l, g\))  
\(\rho_j\) = density of phase \(j\) (\(j = l, g\)) (lbm/ft\(^3\))  
\(\mu_{\text{int}}\) = viscosity of phase \(j\) (\(j = l, g\)) (cp)  
\(\Gamma_{\text{int}}\) = interphase mass influx (lbm/ft\(^3\) s)  
\(\Gamma_{\text{for}}\) = formation of mass influx (lbm/ft\(^3\) s)  
\(\phi\) = liquid composition \(x\)  
\(\lambda\) = source term in the momentum equation (lbf/ft\(^3\))  
\(F_D\) = drag force (lbm/ft\(^3\))  
\(Z_{\text{scv}}\) = position of the center of SCV (ft)  
\(Z_{\text{vcv}}\) = position of the center of VCV (ft)  
\(a_{i,l}\) = velocity coefficient of phase \(j = l, g\) in the momentum equation (lbm/ft\(^3\) s)  
\(a_d\) = coefficient related to the drag force term in the momentum equation (lbm/ft\(^3\) s)  
\(a_{i,l'}\) = velocity coefficient of phase \(j = l, g\) in the momentum equation (lbf/ft\(^3\))  
\(b_1\) = source term in the momentum equation (lbm/ft\(^3\))  
\(G_{i,l'}\) = pressure—velocity correction coefficient (ft/psi s)  
\(G_{i,d'}\) = velocity—velocity correction coefficient  
\(a_{i,l'}\) = coefficient of phase \(j = l, g\) in the overall continuity equation (lbm/ft\(^3\))  
\(b_{i,l'}\) = coefficient of phase \(j = l, g\) in the overall continuity equation (lbm/ft\(^3\) s)  
\(a_{i,l}\) = coefficient of liquid phase in the hold-up equation (lbm/ft\(^3\) s)  
\(b_{i,l}\) = coefficient of liquid phase in the hold-up equation (lbm/ft\(^3\) s)  
\(K_{\text{pre}}\) = precipitation kinetic constant (1/s)  
\(K_{\text{dis}}\) = dissolution kinetic constant (1/s)  
\(K_{\text{agg}}\) = aggregation kinetic constant (1/s)  
\(K_{\text{dep}}\) = deposition kinetic constant (1/s)  
\(C_{\text{pre}}\) = concentration of precipitated asphaltene in the liquid phase (lbm/ft\(^3\))  
\(C_{\text{dis}}\) = actual concentration of dissolved asphaltene in the liquid phase (lbm/ft\(^3\))  
\(C_{\text{eq}}\) = concentration of dissolved asphaltene in the liquid phase at the thermodynamic equilibrium (lbm/ft\(^3\))  
\(R_{\text{pre}}\) = asphaltene precipitation rate (lbm/ft\(^3\) s)  
\(R_{\text{dep}}\) = asphaltene deposition rate (lbm/ft\(^3\) s)  
\(R_{\text{agg}}\) = asphaltene aggregation rate (lbm/ft\(^3\) s)

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