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Compositional Simulation Using the Advanced Peng-Robinson Equation of State

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Abstract

During compositional reservoir simulations where underground fluid composition strongly affects the modeling of recovery processes, flash calculations are commonly employed to help determine the correct number of equilibrium phases, the corresponding compositions, and the phase amount of each phase.

Cubic equations of state (EOS) are widely used in the representation of volumetric and phase equilibria due to their simplicity and solvability. Commonly used cubic EOS such as Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) have well known limitations in predicting liquid phase properties for polar compounds.

In this paper, we present a compositional reservoir simulator equipped with the advanced Peng-Robinson EOS and an efficient and robust multiphase flash algorithm that can accurately predict the phase equilibrium. This method utilizes Michelsen's stability test (Michelsen, 1982) and a combination of accelerated successive substitution and a minimum-variable Newton-Raphson (MVNR) method for fast convergence.

The advanced Peng-Robinson (APR) EOS adds volume translation and a flexible attractive temperature-dependent term to the original PR EOS for accurate PVT and saturation property correlation for polar compounds. Examples of pure compounds and mixtures are tested. Computational results show that the developed simulator provides a more detailed description and better understanding of complex dynamic underground fluid phase behavior that may occur during oil recovery processes.

Introduction

Compositional models are commonly used to simulate complex multiphase flow in a reservoir where phase compositions at equilibrium change with space and time, and an equation of state (EOS) is employed in the models to determine the correct number of equilibrium phases and the corresponding compositions in each phase in each grid block.

Since the late 1970s, many isothermal compositional models using cubic equations of state and taking into account up to three phases (water, gas and oil) have been developed. They are different in how the primary equations and unknowns are selected (Cao, 1999). Fussell and Fussell (1979) published a technique which used a minimum variable Newton-Raphson method to solve a system consisting of fugacity equations and a saturation constraint equation for primary variables: pressure, liquid phase mole fraction, liquid phase composition or pressure, vapor phase mole fraction, and vapor phase composition. Coats (1980) described a fully implicit compositional model which solved material balance equations for hydrocarbon components and water simultaneously. Nghiem et al. (1981) developed an implicit-pressure, explicit-composition, and explicit-saturation model with an EOS. These equations were solved using an iterative-sequential method. Pressure was first obtained by solving a material balance equation and the other unknowns were updated thereafter. Young and Stephenson (1983) presented a more efficient Newton-Raphson method-based procedure which differed from Fussell and Fussell's in the ordering of the equations and unknowns. In summary, a fully implicit model provides better stability; it, however, requires higher computational cost. For a partially implicit model, the implicitness varies with the selection of primary unknowns to be solved for and the choice of reasonable time steps becomes the key point in controlling convergence of the Newton-Raphson iteration and accelerating simulation process (Chen et al., 2006).

In compositional reservoir simulation, an EOS plays a critical role in the representation of volumetric, thermodynamic, and phase equilibrium properties. Since van der Waals first presented his EOS in 1873, a lot of modifications have been presented in the literature. Among these equations, Soave-Redlich-Kwong (Soave, 1972) and Peng-Robinson (1976) equations of state are most popularly used in the petroleum industry due to their simplicity, solvability, and generalization. However, PR and SRK EOS have well known limitations in predicting liquid phase properties especially for polar mixtures. Based on the ideas of Peneloux (1982) and Mathias et al. (1988), Virtual Material Group, Inc. (VMG) implemented an advanced Peng-Robinson

(APR) model in their phase package that adds volume translation and a flexible attractive temperature dependent term into the classical PR EOS in their commercial process simulation software. This model gives more accurate liquid phase property estimation. The package is equipped with a robust flash calculation algorithm which can predict up to three-phase equilibrium based on Michelson's stability test and a combination of accelerated successive substitution and a minimum-variable Newton-Raphson method for fast convergence.

In this paper, based on the modification of Nghiem et al's formulation, we present an implicit-pressure, explicit-composition, and explicit-saturation compositional model using the APR EOS which is able to handle up to three-phase (water-rich, gas and oil), multi-component flow in porous media. The model provides a more detailed description and better understanding of complex dynamic underground fluid phase behavior that may occur during heavy oil recovery processes.

Equation of State and Flash Calculation

The simplest way to determine phase composition in equilibrium is the equilibrium ratio (K-value) approach. However, this approach may predict inaccurate results, and the use of different K-value correlations brings inconsistency in a critical region. Models using an EOS for phase equilibrium and property calculation avoid these computational problems. For example, the PR EOS was developed to predict better liquid densities than the SRK EOS as well as better vapor pressures for hydrocarbons. However, for polar compounds, the PR EOS does not provide an accurate liquid density prediction. Therefore, VMG implemented further modifications in their APR EOS which has all the characteristics of the classic PR EOS. This new EOS adds volume translation and uses a special mixing rule for the calculation of excess volume translations to provide accurate calculation of mixture densities (Users Manual, Virtual Material Group Inc., 2002).

Advanced-Peng-Robinson Equation of State

In 1976, Peng and Robinson developed their two constant cubic EOS

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

in which the attraction parameter $a(T)$ and co-volume parameter b of the mixture are determined by using the mixing rules

$$a = \sum_{m=1}^{N_c} \sum_{n=1}^{N_c} x_m x_n (1 - k_{mn}) \sqrt{a_m a_n} \quad (2)$$

and

$$b = \sum_{m=1}^{N_c} x_m b_m \quad (3)$$

where k_{mn} is the binary interaction parameter between components m and n , and a_m and b_m are the attraction parameter and co-volume parameter for the pure component m . Applying the criteria of criticality, we have

$$a_m = 0.45724 \cdot \alpha_m \frac{R^2 T_{cm}^2}{p_{cm}}, \quad b_m = 0.077796 \frac{RT_{cm}}{p_{cm}} \quad (4)$$

where R is the universal gas constant, and α_m is a temperature dependent parameter given by

$$\alpha_m = \left(1 + \lambda_m \left(1 - \sqrt{\frac{T}{T_{cm}}}\right)\right)^2 \quad (5)$$

$$\lambda = \begin{cases} 0.37464 + 1.5423\omega_m - 0.26992\omega_m^2 & \omega_m < 0.5215 \\ 0.3796 + 1.485\omega_m - 0.1644\omega_m^2 + 0.01666\omega_m^3 & \text{otherwise} \end{cases} \quad (6)$$

The accentric factor ω_m for component m measures the deviation of the molecular shape from spherically symmetric structure. Introducing

$$A = \frac{a \cdot p}{R^2 T^2} \quad \text{and} \quad B = \frac{b \cdot p}{RT} \quad (7)$$

Eq. (1) can be re-written as a cubic equation in terms of the compressibility factor $Z = pv/RT$,

$$Z^3 - (1-B)Z^2 + (A-2B-3B^2)Z - (AB-B^2-B^3) = 0 \quad (8)$$

Then the fugacity of component m in phase α can be evaluated by

$$\ln \frac{f_{m\alpha}}{x_{m\alpha} p_\alpha} = \frac{b_m}{b_\alpha} (Z_\alpha - 1) - \ln(Z_\alpha - B_\alpha) - \frac{A_\alpha}{2\sqrt{2}B_\alpha} \left(\frac{2}{a_\alpha} \sum_{n=1}^{N_c} x_{n\alpha} (1 - k_{mn}) \sqrt{a_m a_n} - \frac{b_n}{b_\alpha} \right) \ln \frac{Z_\alpha + (1 + \sqrt{2})B_\alpha}{Z_\alpha + (1 - \sqrt{2})B_\alpha} \quad (9)$$

Although it was reported that the PR EOS maintains simplicity and provides a better liquid phase density prediction than the SRK equation (Peng and Robinson, 1976), both of them have well known limitations in predicting liquid phase properties for polar compounds. Peneloux and Rauzy (1982) proposed a consistent volume correction for the SRK EOS to improve

volume predictions. The method introduces translations along the volume axis without changing the predicted phase equilibrium conditions. In the APR EOS, further modifications suggested by Mathias et al. (1988) and a special mixing rule for the calculation of excess volume translations are utilized. These modifications provide an improvement in the calculation of both liquid and vapor densities and are necessary in the vicinity of a critical point. The corrected volume is given by

$$v^{corr} = v + s + f_c \left(\frac{0.41}{0.41 + \delta_b} \right), \quad (10)$$

where the bulk modulus δ_b is a dimensionless quantity related to the inverse of the isothermal compressibility

$$\delta_b = -\frac{v^2}{RT} \left(\frac{\partial p}{\partial v} \right)_T, \quad (11)$$

and f_c is chosen to match the true critical volume

$$f_c = v_c - (3.946b + s). \quad (12)$$

Mathias et al. (1988) proposed their simplest possible mixing rule for s and v_c

$$s = \sum_{m=1}^{N_c} x_m s_m \quad \text{and} \quad v_c = \sum_{m=1}^{N_c} x_m v_{cm}, \quad (13)$$

and the corresponding corrections for common hydrocarbon and polar components were listed as well. In the APR EOS, a special mixing rule for the calculation of excess volume translations is used:

$$s_{mix} = \sum_{m=1}^{N_c} s_m x_m + s^{Excess}(T, \bar{x}), \quad (14)$$

thus allowing the calculation of accurate mixture densities.

Flash Calculation

A fast and robust phase equilibrium flash calculation algorithm employed in a compositional model helps to determine the right number of phases and their corresponding composition. A successive substitution method was used by most simulators in the early days. This method is stable but its convergence is slow when the given condition is near a critical region. Fussel and Yanosik (1978) proposed a minimum variable Newton-Raphson iterative method whose convergence is quadratic. However, it requires calculating a Jacobian matrix and its inverse in each step. Mehra et al. (1983) published an accelerated successive substitution algorithm by choosing an optimal step length and their results showed a significant reduction in the number of iterations for convergence. Nghiem et al (1983) combined successive substitution and Powell's hybrid methods and established criteria for efficiently switching; their method possesses the virtues of both stability and robustness.

Since the fugacity equality for each component in each phase is only a necessary but not sufficient condition for phase equilibrium, it may provide wrong equilibrium results without a good initial guess of the iteration. Based on the tangent plane criteria (Baker, et al., 1981), Michelsen (1982) developed a stability test algorithm which not only checks if the phase splitting calculation results are thermodynamically stable and so Gibbs energy is globally minimized, but also provides a very good initial guess for the next flash if necessary. In this work, we utilize Michelsen's stability test and a combination of accelerated successive substitution and the Newton-Raphson method for fast convergence.

Basic Equations

The governing equations of a multiphase, multi-component compositional flow in porous media are derived from the following physical relations: (1) material balance, (2) phase equilibrium conditions, and (3) saturation and composition constraints (Chen, 2007).

Material Balance Equations

Consider a three-phase system (water-rich, gas and oil) that consists of N_c components, water is treated as a component and involved in the flash calculation, we have the material balance equation incorporated with Darcy's law for each component,

$$V_b \left(\frac{\partial \left(\varphi z_m \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)}{\partial t} - \nabla \cdot \left(\sum_{\alpha=w,g,o} x_{m\alpha} \rho_\alpha \frac{K \cdot k_{r\alpha}}{\mu_\alpha} \nabla (p_o - p_{cao} - \gamma_\alpha D) \right) \right) = q_m \quad m = 1, \dots, N_c \quad (15)$$

where φ is the porosity of the porous medium, V_b is the volume of a grid block, $x_{m\alpha}$ is the mole fraction of component m in phase α , and S_α , μ_α and ρ_α are the saturation, viscosity and molar density of phase α respectively. The oil phase pressure p_o is the primary unknown in these equations and the pressure in the other phase is related by the capillary pressure. The molar flow rate q_m of component m is either defined by a constant rate or a constant pressure. For a constant-pressure well, the molar flow rate is given by

$$q_m = \text{PI} \left(\sum_{\alpha=w,g,o} x_{m\alpha} \rho_\alpha \frac{K \cdot k_{r\alpha}}{\mu_\alpha} \right) (p_{bh} - p_{ob}) \quad m=1, \dots, N_c, \quad (16)$$

where p_{bh} is the bottomhole pressure and p_{ob} is the oil pressure in the grid block where the well is located.

Phase Equilibrium Equations

Since mass interchange between phases happens much more rapidly than the fluid flow in porous media, it is physically reasonable to assume that all phases are in equilibria. From the thermodynamic point of view, at given pressure and temperature, the composition of phases in equilibria should satisfy the condition that the Gibbs free energy of the compositional system reaches minimum whose necessary condition is the equality of the component fugacity in each phase,

$$f_{mw} = f_{mg}, \quad f_{mg} = f_{mo} \quad m=1, \dots, N_c, \quad (17)$$

where the fugacity $f_{m\alpha}$ is defined by the EOS selected.

Constraint Equations

The saturation constraint and component mole fraction balance imply

$$S_w + S_g + S_o = 1, \quad (18)$$

$$\sum_{m=1}^{N_c} z_m = \sum_{m=1}^{N_c} x_{mw} = \sum_{m=1}^{N_c} x_{mg} = \sum_{m=1}^{N_c} x_{mo} = 1, \quad (19)$$

and the phase mole fraction constraint gives

$$W + V + L = 1. \quad (20)$$

Other Relationships

Material balances on the phases hold for all components

$$z_m = W \cdot x_{mw} + V \cdot x_{mg} + L \cdot x_{mo}, \quad (21)$$

The phase mole fractions and saturations are related by the following equations:

$$W = \frac{\rho_w S_w}{\rho_w S_w + \rho_g S_g + \rho_o S_o}, \quad (22)$$

$$V = \frac{\rho_g S_g}{\rho_w S_w + \rho_g S_g + \rho_o S_o}, \quad (23)$$

and

$$L = \frac{\rho_o S_o}{\rho_w S_w + \rho_g S_g + \rho_o S_o}. \quad (24)$$

Solution Algorithms

We solve the pressure equations using the finite difference method. The capillary pressures are assumed unchanged during the iteration. Once $p_o^{(k+1)}$, a new iterate of p_o is obtained, the feed composition z is updated. Then flash calculations are performed to find the component mole fraction $x_{m\alpha}^{(k+1)}$, phase mole fraction $W^{(k+1)}$, $V^{(k+1)}$ and $L^{(k+1)}$, molar density $\rho_\alpha^{(k+1)}$, and viscosity $\mu_\alpha^{(k+1)}$. The iteration is repeated until convergence.

Difference Equations

The material balance equation (15) can be written in the difference form. By introducing the transmissibility of phase α ,

$$T_\alpha = \frac{A_c}{\Delta l} \frac{K \cdot k_{r\alpha}}{\mu_\alpha} \rho_\alpha, \quad (25)$$

we obtain the equivalent difference equation,

$$\frac{V_b}{\Delta t} \left[\left(\varphi z_m \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)^{n+1} - \left(\varphi z_m \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)^n \right] - \Delta \left(\sum_{\alpha=w,g,o} T_\alpha^n x_{m\alpha}^n (\Delta p_o^{n+1} + \Delta p_{cao}^n - \gamma_\alpha^n \Delta z) \right) - q_m = 0 \quad m = 1, \dots, N_c. \quad (26)$$

Summing Eq. (26) over N_c components, we obtain the pressure equation at the n th time step

$$\frac{V_b}{\Delta t} \left[\left(\varphi \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)^{n+1} - \left(\varphi \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)^n \right] - \Delta \left(\sum_{\alpha=w,g,o} T_\alpha^n (\Delta p_o^{n+1} + \Delta p_{cao}^n - \gamma_\alpha^n \Delta z) \right) - q_h = 0 \quad (27)$$

where

$$q_h = \sum_{m=1}^{N_c} q_m \quad (28)$$

Jacobian Matrix for Pressure Equation

The pressure equation is solved by the Newton-Raphson method where the Jacobian matrix needs be calculated in each iteration step. Let $\vec{r}^{(k)}$ be the residual of Eq. (27) at the k th iteration; the new iterate values for p_o are obtained from

$$\vec{p}_o^{(k+1)} = \vec{p}_o^{(k)} + \delta \vec{p}_o^{(k+1)} \quad (29)$$

where $\delta \vec{p}_o^{(k+1)}$ is a solution of

$$J^{(k)} \cdot \delta \vec{p}_o^{(k+1)} = -\vec{r}^{(k)} \quad (30)$$

In Cartesian coordinates, the Jacobian matrix is tri-diagonal for one-dimensional problems, penta-diagonal for two-dimensional problems, and hepta-diagonal for three-dimensional problems. Its off-diagonal and diagonal elements can be evaluated by

$$J_{ij}^{(k)} = \left(\sum_{\alpha=w,g,o} T_\alpha \right)_{\frac{i+j}{2}}^{(k)} \quad (31)$$

and

$$J_{ii}^{(k)} = - \left(\sum_{\alpha=w,g,o} T_\alpha \right)_{\frac{i+j}{2}}^{(k)} + \left(\frac{\partial q_h}{\partial p_o} \right)_{\frac{i+j}{2}}^{(k)} - \frac{V_b}{\Delta t} \left(\frac{\partial \left(\varphi \sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right)}{\partial p_o} \right)_i^{(k)} \quad (32)$$

where $(i + j)/2$ stands for the link between the i th and j th grid blocks. Ngheim et al. (1981) suggested that the derivative of the accumulation term with respect to pressure can be approximated by neglecting the saturation variation as pressure changes

$$\left(\frac{\partial \left(\varphi \sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right)}{\partial p_o} \right)_i^{(k)} = \left(\frac{\partial \varphi}{\partial p_o} \left(\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right) + \varphi \sum_{\alpha=w,g,o} \left(S_\alpha \frac{\partial \rho_\alpha}{\partial p_o} \right) \right)_i^{(k)} \quad (33)$$

where $\partial \varphi / \partial p_o$ and $\partial \rho_\alpha / \partial p_o$ are given by

$$\frac{\partial \varphi}{\partial p_o} = \varphi_r c_f \quad \text{and} \quad \frac{\partial \rho_\alpha}{\partial p_o} = \frac{1}{RTZ_\alpha} \left(1 - \frac{p_o}{Z_\alpha} \frac{\partial Z_\alpha}{\partial p_o} \right) \quad (34)$$

Then, Eq. (30) can be solved by Gauss elimination if the system is small; for a large system, an iterative method for a sparse system is preferred (Saad, 2002).

Composition and Saturations

Once a new iterate value of pressure is obtained, the feed composition and water saturation in each grid block can be updated explicitly by solving Eq. (26):

$$z_m^{(k+1)} = \frac{\Delta \left(\sum_{\alpha=w,g,o} T_\alpha^n x_{m\alpha}^n (\Delta p_o^{(k+1)} + \Delta p_{cao}^n - \gamma_\alpha^n \Delta z) \right) + q_m + \frac{V_b}{\Delta t} \left(\phi z_m \left[\sum_{\alpha=w,g,o} S_\alpha \rho_\alpha \right] \right)^n}{\Delta \left(\sum_{\alpha=w,g,o} T_\alpha^n (\Delta p_o^{(k+1)} - \Delta p_{cao}^n - \gamma_\alpha^n \Delta z) \right) + q_h + \frac{V_b}{\Delta t} \left(\phi \sum_{\alpha=w,g,o} x_{i\alpha} \rho_\alpha S_\alpha \right)^n} \quad (35)$$

The terms

$$\frac{k_{r\alpha} \rho_\alpha}{\mu_\alpha} x_{m\alpha} \quad \alpha = w, g, o$$

are evaluated using upstream weighting.

A flash calculation is performed on $\vec{z}^{(k+1)}$ and at $p_o^{(l+1)}$ to find the component mole fraction $x_{m\alpha}^{(k+1)}$ in each phase, the phase mole fraction $W^{(k+1)}$, $V^{(k+1)}$ and $L^{(k+1)}$, and the phase molar density $\rho_\alpha^{(k+1)}$. The phase viscosity $\mu_\alpha^{(k+1)}$ is returned from the flash package as well. The saturations of gas, oil and water can be computed by using the following formulas,

$$S_g^{(k+1)} = \left(\frac{1}{1 + \frac{L\rho_g}{V\rho_o} + \frac{W\rho_g}{V\rho_w}} \right)^{(k+1)} \quad (36)$$

$$S_o^{(k+1)} = \left(\frac{1}{1 + \frac{V\rho_o}{L\rho_g} + \frac{W\rho_o}{L\rho_w}} \right)^{(k+1)} \quad (37)$$

and

$$S_w^{(k+1)} = 1 - S_g^{(k+1)} - S_o^{(k+1)} \quad (38)$$

The whole workflow of the procedure is illustrated in **Fig. 1**.

Examples

A few examples including liquid density prediction for pure component, mixture and compositional reservoir simulation using APR EOS are studied, and satisfactory results are obtained.

Liquid Density Prediction

This example tests liquid density predictions of saturated water and water-methanol system, and they were reported by Mathias et al. as well (1988). The data for comparison come from the International Association for the Properties of Water and Steam (IAPWS) Industrial Formulation 1997 (Wanger et al., 2000), and Friedman and Sherage's paper (Friedman and Sherage, 1965) and the plots of the calculated liquid density using the PR and APR EOS are shown in **Figs. 2** and **3**. Blue line and green dots represent the densities prediction calculated from APR and PR EOS, respectively, and red circles are experimental data. From these plots we can find that the PR EOS works well for the vapor phase but fairly underestimates the liquid density, which is improved by the APR EOS. It is evident that the APR EOS provides very reasonable results for density prediction for both the pure compound and mixture.

One-Dimensional Miscible Flooding Simulation

In this example, Coats' one-dimensional miscible flooding data (**Table 1**) is used. The size of the reservoir is 250 feet in length, 100 feet in width and 50 feet in thickness. The initial reservoir pressure is 2,000 psia and reservoir temperature is 160 °F. The initial oil composition in the reservoir is 20% methane, 20% n-butane and 60% n-decane. The capillary pressure and gravity are neglected. 100 MSCF (263 lb-mole) gas consists of 68.4% methane and 31.6% n-butane is injected per day. The bottomhole pressure for production is 2,000 psia (Coats, 1980). The reservoir is discretized into 20 grid blocks and time step of 3.75 days is specified.

Gas saturation profile vs. dimensionless is plotted in **Fig. 4**. Two runs using PR EOS and APR EOS are performed for comparison purpose. Gas saturation predicted by the model using PR EOS exactly matches Coats' result. Calculated miscible front is located between 0.1 and 0.2 in dimensionless distance. The miscible front predicted by APR model is a bit more advance than what PR model predicts and so is the location of two-phase zone. Corrected density prediction using APR EOS also results in slight difference in calculated composition profiles and phase densities. As is shown in **Fig. 5**, APR model has higher methane mole fraction and lower n-decane mole fraction prediction while the oil phase density calculated by APR model is higher as well (**Fig. 6**), since PR EOS underestimates liquid density. The plots are consistent with our observation from the previous example, and better liquid prediction makes the compositional model equipped with APR EOS more accurate in simulation results.

Conclusions

In this paper, we present an implicit pressure explicit composition and saturation compositional model using the APR EOS. It improves liquid density prediction and provides accurate PVT and saturation property correlation for polar compounds by adding volume translation and a flexible attractive term temperature dependency to the original PR EOS. Computational results show that the developed simulator provides a more detailed description and better understanding of complex dynamic underground fluid phase behavior that may occur during oil recovery processes.

Nomenclature

$a(T)$	=	attraction parameter
A_c	=	cross-sectional area perpendicular to flow
b	=	co-volume parameter
c_r	=	rock compressibility
D	=	depth
f	=	fugacity
J	=	Jacobian matrix
K	=	permeability
k_{mn}	=	interaction parameter between components m and n
k_r	=	relative permeability
k_{rgcw}	=	relative permeability to gas at connate water
k_{rocw}	=	relative permeability to oil at connate water
n_g, n_o	=	exponents on relative permeability curves
Δl	=	space difference
L	=	mole fraction of oil phase
N_c	=	number of components
p	=	pressure
p_{bh}	=	bottomhole pressure
p_o	=	oil phase pressure
p_{cao}	=	capillary pressure between phase α and oil phase
PI	=	productivity index
q_m	=	mole flow rate of component m
q_h	=	overall mole flow rate
R	=	universal gas constant
s	=	molar volume correction term
s^{Excess}	=	excess volume translation
S_α	=	saturation of phase α
S_{gc}	=	critical gas saturation
S_{gr}	=	residual gas saturation
S_{org}	=	residual oil saturation to gas
S_{orw}	=	residual oil saturation to water
t	=	time
Δt	=	time step
T	=	temperature
T_c	=	critical temperature
T_α	=	transmissibility of phase α
v	=	molar volume
v_c	=	critical volume
v^{corr}	=	corrected molar volume
V	=	mole fraction of gas phase
V_b	=	grid block volume
W	=	mole fraction of water-rich phase
$x_{m\alpha}$	=	mole fraction of component m in phase α
Z_α	=	compressibility factor of phase α
γ_α	=	specific weight of phase α
δ, Δ	=	difference operator
δ_b	=	buck modulus
μ_α	=	viscosity of phase α
ρ_α	=	molar density of phase α
φ	=	porosity
ω	=	acentric factor

Superscripts

(k)	=	number of iterations
n	=	number of time step

Subscripts

c	=	critical
g	=	gas phase
i, j	=	grid block indices
m, n	=	component indices
o	=	oil phase
w	=	water-rich phase
α	=	phase index

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Table 1 – Data for 1D miscible flooding model	
Reservoir dimensions (ft) length, width, thickness	250, 100, 50
Initial Pressure (psi)	2000
Reservoir Temperature (°F)	160
Permeability (md)	2000
Porosity	0.2
Rock compressibility (psi ⁻¹)	4×10^{-6}
Water compressibility (psi ⁻¹)	3×10^{-6}
Initial Saturation S_w, S_{g1}, S_o	0.2, 0, 0.8
Initial Composition C_1, nC_4, nC_{10}	0.2, 0.2, 0.6
Capillary pressure (psi)	0
Relative permeability data	
S_{wc}	0.2
S_{org}	0.2
S_{gc}	0
S_{gr}	0.15
K_{rocw}	1
K_{rgcw}	1
k_{rw}	0
n_l	7
$n_{og}=n_g$	2
Injection Rate (MSCF/day)	100
Injected composition C_1, nC_4, nC_{10}	0.684, 0.316, 0
Productivity index (ft ³ -cp/day-psi)	1.012×10^5
Production pressure (psi)	2000

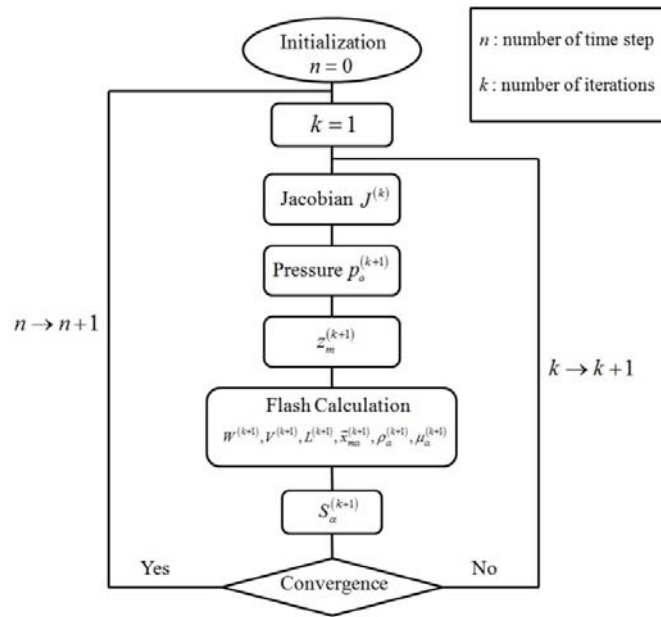


Fig. 1 – Flow chart for iterative procedure.

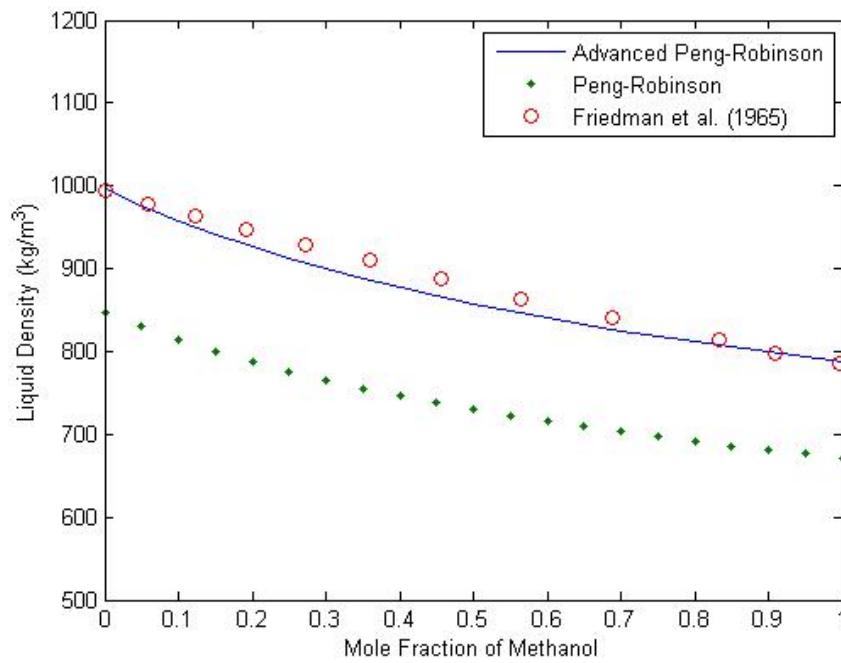


Fig. 2 – Liquid density of water-methanol system (T = 25°C, P = 101.325 kPa).

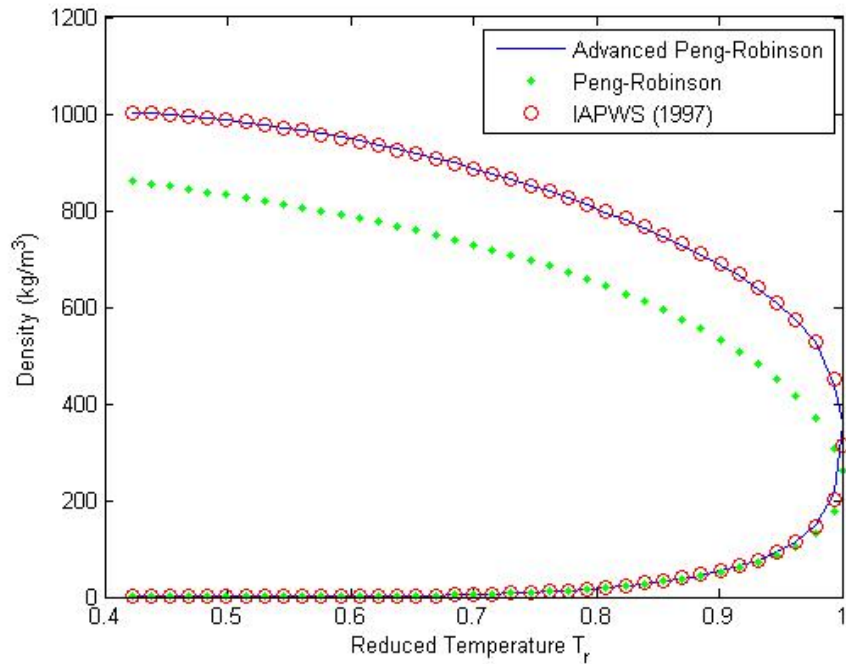


Fig. 3 – Prediction of density for saturated water.

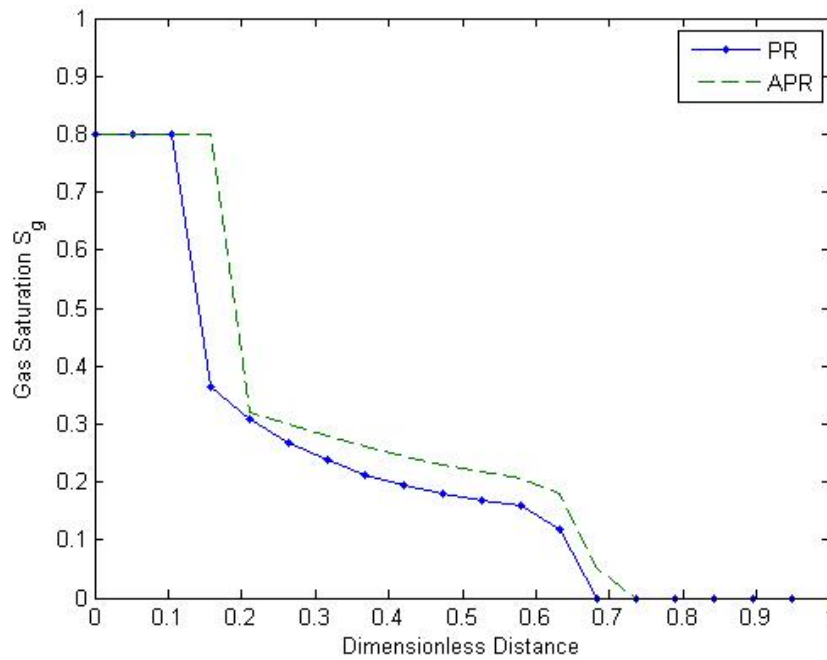


Fig. 4 – Gas saturation vs. dimensional distance.

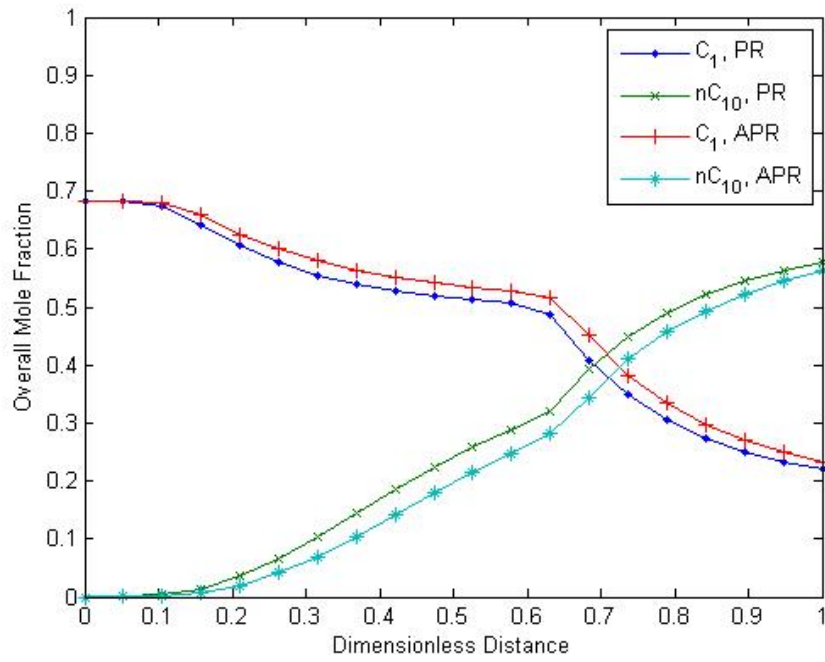


Fig. 5 – Overall composition vs. dimensionless distance.

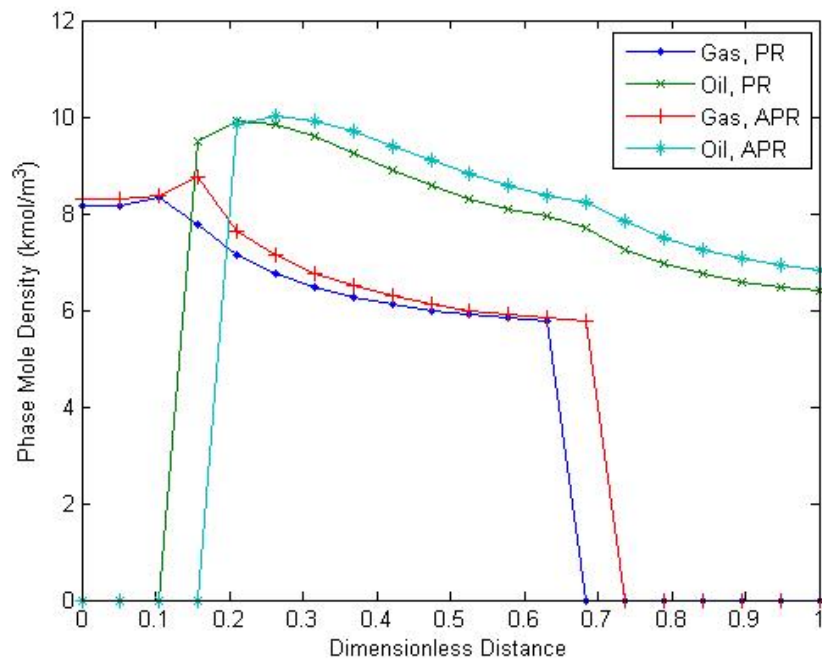


Fig. 6 – Phase density vs. dimensionless distance.