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Summary

Understanding the thermodynamic behavior of each flowing phase in a petroleum reservoir allows for accurate quantification of these phases. This work explains how to develop and run a thermodynamic model to reliably forecast the equilibrium behavior of oil-gas-brine systems across a reasonable pressure and temperature range. The 3-phase negative flash method is tested against previously published data in the literature. The multiphase flash approach is used to develop linearized physical operators utilizing an Operator Based Linearization (OBL) modeling technique that allows for the nonlinear solution of governing equations to include various complicated physics. To our knowledge, this is the first implementation to the coupling of 3-phase flash calculations for hydrocarbons and brines have been using fugacity-activity models with a a sophisticated, high-efficiency linearization technique. Such coupling improves the efficiency and flexibility of physical phenomena modeling of the fluid flow in porous subsurface reservoirs.

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Summary

Understanding the thermodynamic behavior of each flowing phase in a petroleum reservoir allows for accurate quantification of these phases. This work explains how to develop and run a thermodynamic model to reliably forecast the equilibrium behavior of oil-gas-brine systems across a reasonable pressure and temperature range. The 3-phase negative flash method is tested against previously published data in the literature. The multiphase flash approach is used to develop linearized physical operators utilizing an Operator Based Linearization (OBL) modeling technique that allows for the nonlinear solution of governing equations to include various complicated physics. To our knowledge, this is the first implementation to the coupling of 3-phase flash calculations for hydrocarbons and brines have been using fugacity-activity models with a a sophisticated, high-efficiency linearization technique. Such coupling improves the efficiency and flexibility of physical phenomena modeling of the fluid flow in porous subsurface reservoirs.

Introduction

The hydrocarbon recovery from enhanced oil recovery (EOR) processes accounts for 2% of global oil production nowadays (IEA, 2020). Currently, engineers have access to new technology that provides better understanding of the complex physics in the subsurface reservoirs, thus developing many mature fields into producing sectors. However, there are challenges to implementing EOR, such as interactions between carbon dioxide and hydrocarbons, which highlight the need of multiphase equilibria when vapor-liquid-liquid equilibrium is experienced (Massarweh 2020,2021).

The presence of water has a slight impact on the phase behavior of the reservoir mixtures in an isothermal setting, although it's always present. However, high temperature conditions give rise to challenging behavior in systems with high water content. Furthermore, the cost of performing three phase flash calculations can be computationally arduous for large numbers of grid cells, as the stability test and flash calculations demand high cost in the molar variable formulation and cannot be skipped. The set of conservation equations at each global nonlinear iteration requires closure through local thermodynamic constrains. Using constant K-values approach in this case lowers the cost of the flash computations massively. Moreover, free-water flash approach is utilized to simplify the assumptions regarding phase compositions, and hence reduce the computational cost but might have adverse effect on the consistency of the results.

In this work, we focus on developing a rigorous multiphase equilibrium flash model for carbon dioxide injection in enhanced oil recovery applications. The main aim of the study is to present a rigorous multiphase flash procedure based on combination of conventional Equation of State, Henry's law and Activity models to account for the presence of salts while incorporating efficient stability and negative flash procedure coupled with high order linearization and discretization schemes that lead to acceptable results with low computational costs in reservoir simulations.

Method and/or Theory

The use of an EoS-based model allows for a more precise determination of aqueous phase behavior. The most difficult part of estimating the phase split is figuring out how many phases are present in a combination at a given temperature and pressure. Typically, an explicit analysis of Michelsen's stability test (Baker, Pierce & Luks, 1982; Michelsen, 1982 a,b) is used to find the stationary points. The solution at these places is utilized to establish the system's stability, but to prevent missing any instability zones, several initial estimations of the equilibrium ratio (K) are required.

The thermodynamic equilibrium in a three-phase system is achieved when the fugacity of each component in each phase is equal,

$$f_i^V = f_i^L = f_i^{Aq} \tag{1}$$

where f_i is the fugacity of the vapor (V), liquid (L), or aqueous (Aq) phase, and i is the index of the component. The fugacity coefficient in the vapor and the liquid phases is typically calculated using a traditional equation of state approach such the Peng-Robinson EOS,

$$\ln \phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B) - \frac{1}{\delta_2 - \delta_1}\frac{A}{B}\left(\frac{2a_{ij}}{a} - \frac{b_i}{b}\right)\ln\left(\frac{Z+\delta_2 B}{Z+\delta_1 B}\right) \tag{2}$$

where δ_1 and δ_2 are empirical constant for PR-EOS defined as 1-√2 and 1+√2 respectively, a and b are empirical constants related to temperature and pressure, a_{ij} is the composition dependent mixing rule, and Z is the compressibility factors. For more details on the formulation of these parameters, we refer the reader to the original paper of Peng and Robinson.

The fugacity coefficient in the aqueous phase is however calculated using a Henry's law model. The water-rich phase is modelled using an activity model that is based on Henry's law constants. The fugacity of the aqueous phase is reported in (Spycher & Pruess, 2005) as,

$$f_i^{aq} = w_i H_i \gamma_i \tag{3}$$

where H_i is henry's constant γ_i is the activity coefficients and w_i is the molar fraction of each component in the aqueous phase.

To account for the divergence of a given mixture from ideality, the activity coefficient is derived using a correlation by (Rogers & Pitzer, 1982). Pitzer's relation holds true in high-salt solutions, which is crucial since activity coefficients are heavily impacted by anions, cations, and particle-pair interactions.

$$\ln \gamma_i = \sum_c 2m_c\lambda_{i-Na} + \sum_c 2m_a\lambda_{i-Cl} + \sum_c\sum_a 2m_a m_c \xi_{i-Na-Cl} \tag{4}$$

where $\mathrm{m_c}$ is the cation molality, $\mathrm{m_a}$ is the anion molality, $\lambda_{\mathrm{i-Na}}$ and $\lambda_{\mathrm{i-Cl}}$ are the second-order parameters representing cations and anions, and $\xi_{\mathrm{i-Na-Cl}}$ is a third order parameter dependent on pressure and temperature.

The flash process is used to guess what each phase of a system is made up of. The unknown variables F_j and x_{ij} indicate the molar ratio of each phase in the system and the mole fraction of a component i in phase j respectively and are typically computed at constant pressure and temperature. If we consider the vapor phase as a reference phase in a three-phase system, the following Richford Rice equations are derived,

$$\sum_{j=1}^{N_c}(x_{il} - x_{iv}) = \sum \frac{(K_{iv} - 1)z_i}{F_v + F_l K_{il} + F_w K_{iw}} = 0 \tag{5}$$

$$\sum_{j=1}^{N_c}(x_{iw} - x_{iv}) = \sum \frac{(K_{iw} - 1)z_i}{F_v + F_l K_{il} + F_w K_{iw}} = 0 \tag{6}$$

where F_l, F_v and F_w denote phase fractions for the liquid, vapor, and aqueous phases respectively.

In the proposed technique, the successive substitution method (SSI) is employed to update and solve both the stability and flash computations. A generalized negative flash approach devised by (Iranshar et al., 2010a) is used to solve the RR equations. Because it allows for a negative phase fraction, this approach can be classified as mathematically abstract. The negative flash procedure along with standard stability testing is utilized when there is a combination of an unknown number of phases. We begin the stability study with an L-W test. The trial and reference phases are determined by the molar percentage of water content in the initial feed; if the feed contains more than 50% water, the aqueous phase is considered as the reference phase, while the liquid phase is handled as the trial phase. An aqueous or liquid phase occurs if the L-W test confirms system stability. The L-W and V-W tests are similar in nature since the fugacities of the vapor and liquid phases are determined using an EOS.

Numerical Analysis Cases

To perform our simulations, we use an innovative and extremely efficient linearization approach called Operator Based Linearization (OBL) to combine the three-phase activity-based flash model with the transport equations in a hydrocarbon reservoir (Voskov, 2017). The conservation of mass, Darcy's law, and an equation of state are the governing equations for multiphase flow of a fluid in a porous media. The diffusion and dispersion forces are believed to be very minor, thus they may be ignored. The following is the continuity equation:

$$F_i = \frac{\partial N_i}{\partial t} + L_i = 0 \tag{7}$$

where F_i is the residual function that should amount to zero after the system to converges to an acceptable solution, $(\partial N_i)/\partial t$ is the accumulation term and L_i is the flux term. The applicability of this equation is broad, as each component can appear in any or all of the three-phase equations. The OBL technique is used to discretize and rewrite the governing equation in terms of state-based (physical properties of fluid and rock) and space-based (properties changed in space) operators.

$$V\phi_0[\alpha_i(\omega) - \alpha_{ci}(\omega_n)] - \Delta t \sum_{l\in L(i)} \sum_{j=1}^{n_p} \left(\Gamma^l \beta_{\mathrm{ij}}^l(\omega)\Delta\Phi_j^l + \Gamma_d^l \gamma_{\mathrm{ij}}^l(\omega)\Delta\varepsilon_{\mathrm{ij}}\right) + \theta(\xi,\omega,u) \quad (8)$$

where ω is a state-dependent parameter and ξ is a space-dependent parameter. The full discussion of the parametrization and linearization of the continuity equation can be found in (Voskov,2017) work. Moreover, the full details of implementing the OBL technique in an advanced parallel framework for reservoir simulation with high order discretization schemes such as Mixed Hybrid Finite Element method (MHFEM) and Mimetic Finite Difference (MFD) is discussed in details in the work of (Abd and Abushaika, 2021; Abd et al., 2021; Nardean et al., 2020; Li et al., 2020; Abushaikha and Terekhov, 2020; Zhang and Abushaikha, 2019 a,b; Hjieij and Abushaika, 2019a,b; Abushaikha et al., 2017) that we refer the reader to.

In the test we present here, we use two distinct meshes (1-D and 2-D) to simulate a CO2 injection situation and project the injection and production profiles onto the ternary diagram of a nC10-CO2-H2O mixture. The initial mesh is in 1-D and consists of 1000 cells in the x-direction, with an injector and a producer at the grid's far ends, and scalar porosity and permeability of 0.3 and 1000 md respectively. The second mesh, on the other hand, is the seventh layer of the SPE-10 model with four producers around the corners and an injector in the center. The mesh is 60x220x1, with a highly heterogeneous porosity and permeability profiles. The 1-D and 2-D models are initialized at pressures of 100 bar and 400 K, respectively. While the producers operate at an average pressure of 80 bar, the injector well injects pure CO2 at 120 bar. The multiphase flash package is used to construct the ternary diagram of the nC10-CO2-H2O mixture at the stated condition (see Fig. 9). On the diagram, the injection and production conditions are represented by red and green dots, respectively.

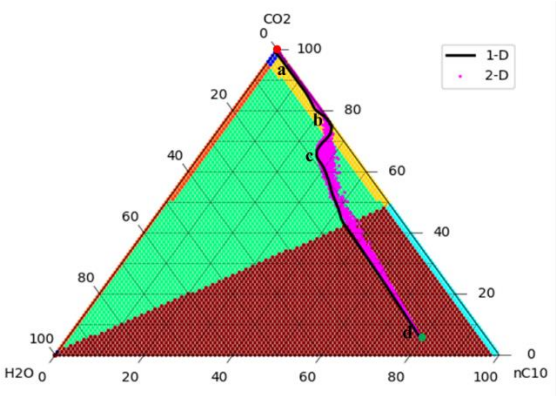

Figure 1 *Ternary phase diagram for a nC10-CO2-H2O system with constant Pressure and Temperature at 100 bar and 400 K respectively. The injection path is drawn between the injection condition (red point) and the initial reservoir condition (green)*

At the end of the simulation, the concentration distribution of each component is plotted versus the distance traveled, as shown in Fig. 3 for the 1-D model. With the locations a, b, c, and d on the ternary diagram exhibiting the principal shocks, we find that composition profiles are essentially identical for both models. The solution path begins with a pure CO2 composition and then transitions to a two-phase (V-L) region with a shock from injection condition. Point b is on a tie line that extends through point a, as shown in Fig. 1. As it approaches the three-phase (V-L-Aq) area, the solution route shifts to the non-tie-line path at point c. After then, the route enters a two-phase (L-Aq) area and reaches point d at initial the reservoir conditions, causing another shock. The concentration maps of Fig. 2 show that the nC10

concentration increases steadily as the solution path is traced from the injection composition to the initial composition upstream where this profile mirrors that of the oil saturation in the reservoir.

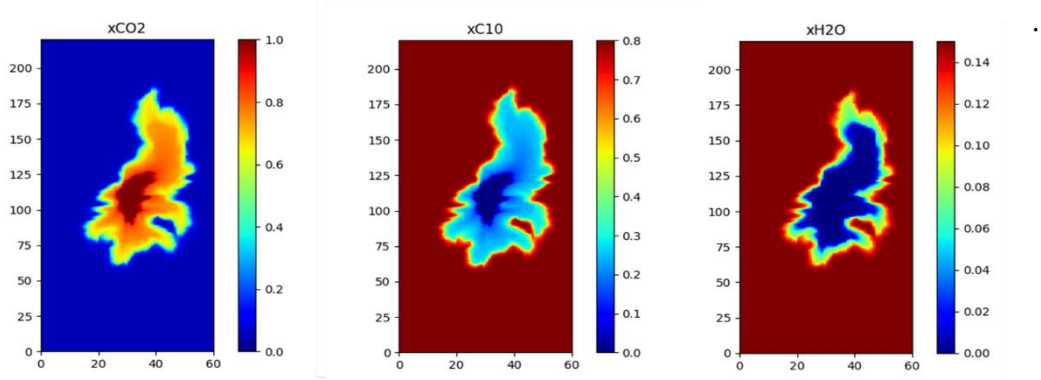

Figure 2 *The saturation maps of the reservoir components at a simulation time of t=3500 days. The flow tends to move to the region of the highest permeability and towards the four producer wells*

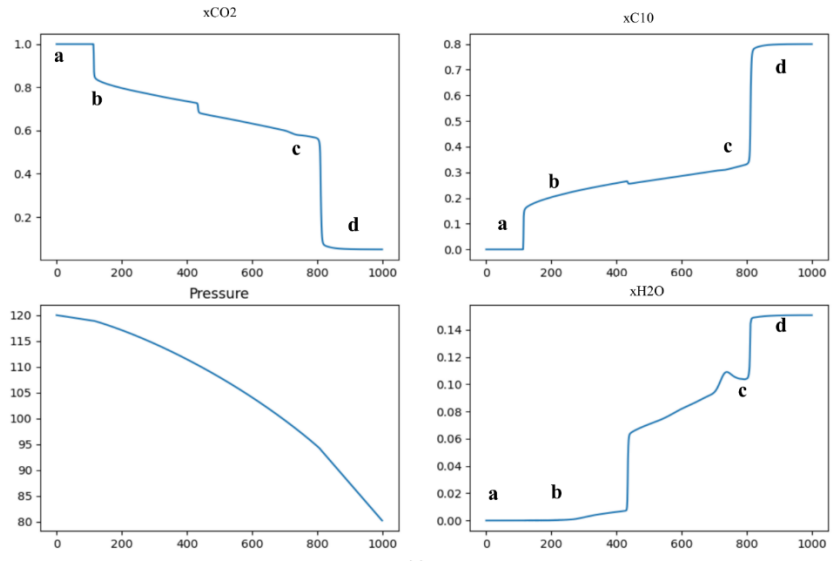

Figure 3 *-The solution profiles of composition and pressure with distance at the end simulation time for (a) 1-D model and (b) 2-D SPE-10 model.*

Conclusions

In a three-phase (Oil/Gas/Water) system, reliable phase behavior prediction requires solving a set of nonlinear equations in a multistage flash scheme with efficient and robust phase stability testing. The number of existing phases in the system may be determined by minimizing the TPD function. If a phase is absent during a three-phase negative flash, the equilibrium phase distribution is determined using a two-phase flash. Data from the literature is used to validate the three-phase negative flash approach. Variations in a mixture's pressure and temperature induce the appearance and disappearance of phases, which the model properly represents. The multiphase flash approach is used to develop linearized physical characteristics utilizing an Operator Based Linearization (OBL) modeling technique that allows the nonlinear solution of governing equations to include numerous complicated physics. In 1-D and 2-D models, the final package is incorporated into a fully implicit reservoir simulator and used to simulate various scenarios of CO2 and H2O injection. The composition concentration profiles and their projection on the ternary diagrams were highly consistent, demonstrating the package's capacity to mimic full-field situations with true petrophysical features.

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