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Non-iterative phase behavior model with application to surfactant flooding and limited compositional simulation☆

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ABSTRACT

Hand's method is typically used to empirically calculate the equilibrium compositions for ternary systems between two liquid phases. Oil field application of Hand's method is generally limited to surfactant phase behavior with oil and brine, primarily because the excess oil and brine phases are nearly immiscible. Hand's method is not accurate to represent liquid–vapor equilibrium, especially as oil and gas become miscible. It also requires iterations, which means there is no guarantee of convergence.

In this paper, we present a new empirical phase behavior model to replace Hand's method. The new method is faster and more accurate, and applicable for both surfactant phase behavior and liquid–vapor equilibrium. The new approach is non-iterative and always finds a tie line or its extension even for the limiting tie line at the critical point. Our approach transforms tie lines to a new compositional space, where all tie lines become parallel. Equilibrium compositions are then easily determined in the transformed space. Besides improved accuracy and robustness, the flash calculations for ternary systems show that the new method is up to 100 times faster than conventional calculations using a cubic equations-of-state (EOS), and up to seven times faster than Hand's method. When incorporated in a compositional simulator, the new method reduces flash calculation time to nearly zero compared to the solution of the pressure/compositional equations. Thus, speedup is proportional to the fraction of time occupied by flash calculations within the simulator. For example, if flash calculations are 50% of total simulation time, speedup is nearly a factor of two using the new approach. This approach is ideally suited for fast recovery estimations for miscible gas floods, and fills the gap between standard or modified black-oil models and fully compositional simulations.

1. Introduction

Phase split calculations are essential to model compositional effects in compositional reservoir simulation, and solubility ratios in surfactant flooding. Compositional modeling with a cubic EOS, however, is computationally intensive and generally requires the use of large grid-block sizes. Because of this limitation, black-oil models are often preferred because of their speed and simplicity. Black-oil models, however, are inaccurate to model displacements where compositional effects are dominant, such as those that occur during gas flooding. A variety of limited compositional models have been developed over the years to fill the gap between black-oil models and fully compositional models, but these often make phase behavior approximations and assumptions that are often inaccurate.

The most widely used limited compositional models fall into three main categories: constant *K*-value models, four-component simulators, and pseudo-ternary compositional models. Constant *K*-value models, such as those of Bolling [1], Whitson [2], and CMG STARS [3] make *K*-values a function of temperature and pressure. These models are generally limited in accuracy to immiscible floods where *K*-values are relatively independent of composition. The second type, four-component simulators, generally adds a solvent component to the standard black-oil models. Many of these also use Todd–Longstaff [4] mixing rules, and/or parameters, such as relative permeability, that change based on whether the pressure is above or below the MMP. These models, however, suffer from the same deficiency of compositional dependence as in black-oil models. Pseudo-ternary compositional models, such as that by Tang and Zick [5], attempt to model both compositional and pressure dependence using only three components: dead oil, dry gas, and solvent. Their model assumes that all tie lines go though the apex of a ternary diagram corresponding to dead oil. They further simplify

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phase behavior by approximating the pressure-dependent dew-point and bubble-point curves by two linear segments that extend to a critical point. These simplifications, although better than previous limited compositional models, are not physical and can lead to inaccuracies in modeling the compositional changes that occur during a displacement of oil by gas.

Another approach that has been used is to speed up fully compositional simulators by introducing reduced parameters (e.g. Michelsen [6], Li and Johns [7], Li [8] and Okuno et al. [9]). The use of reduced parameters can significantly decrease computational time especially when many components are present, but they are still slower than black-oil simulators or limited ternary compositional simulators.

Methods that store tie line information are also available. In CMG STARS, tie-line information (K-values) for a three-component two-phase system at a given pressure and temperature can be stored in a table, where component 1 is the lightest component. For a given overall composition z_1, z_2, and z_3 the Rachford–Rice equation is solved based on interpolation of the K-values from the nearest tie lines at that composition and pressure/temperature pair. Although typically faster than a cubic EOS solution for iso-fugacities, this K-value approach still requires Rachford–Rice iterations and a tie-line search algorithm. It also can suffer in accuracy near critical points, where K-values change rapidly.

Another approach for speed up of two-phase flash calculations is given in VIP [10]. In this approach phase behavior estimated from a cubic EOS is parameterized using the recovery factor of a component. A table of compositions is stored for a given temperature and pressure similar to the approach in CMG STARS. Some of the tie lines are automatically considered based on the initial oil composition, injected gas composition and composition route in PVT tests using an EOS. A search scheme finds the closest overall composition, pressure, and temperature in the tabular data. Once the nearest overall composition is found using a defined tolerance, the recovery factor is used to calculate the equilibrium compositions. The advantage of this method over STARS is that it eliminates the Rachford–Rice step, but still requires a search algorithm and interpolation scheme. It also can fail near critical regions.

Recently, Entov et al. [11] and Voskov and Tchelepi [12] proposed a method based on compositional space parameterization. This method creates a table of equilibrium data and finds the correct tie line using a more advanced search scheme than is implemented in VIP. The tie-line search is limited to the ones that are on the compositional path in a parameterization of the tie-line compositional space. Thus fewer tie lines are checked to satisfy the objective function. Like VIP and STARS, this method requires interpolation when reservoir pressure or temperature changes, and the accuracy of this approach has yet to be determined especially for compositions near the critical region.

An old method for phase behavior description is Hand's method (Hand [13]), which is still used today to represent surfactant flooding with good accuracy (e.g. UTCHEM, Delshad et al. [14,15]). Hands model uses only three components, which for surfactant flooding are surfactant, oil, and brine. Hand's method generally requires iterations for convergence. In the same paper, Hand also proposed the use of a constant transformation factor to transform tie lines so that they become parallel in a new compositional space. This approach, however, is not accurate for vapor–liquid equilibrium, primarily because the slopes of the tie lines change significantly with compositions and thus are not parallel after transformation with a constant transformation factor.

Van-Quy et al. [16] developed a model for liquid–vapor equilibrium using Hand's method to represent a binodal curve. He calculates the tie lines based on a common intersection point, called a pivot point, which can be in negative composition space. His method is inaccurate because equilibrium compositions must lie on the line connecting the overall composition and the pivot point. In addition, his approach is also iterative like that of Hand's method.

This paper develops a new empirical phase behavior model that is more accurate, faster, and completely robust to replace Hand's method. Our approach uses the idea in Hand's original paper of transforming tie lines into a new compositional space so that they become parallel. Our approach differs from his in that we use compositionally dependent transformation factors that accurately match both surfactant and liquid–vapor phase behavior. In addition our method is faster and more robust than those proposed by VIP, CMG STARS, and Voskov and Tchelepi since it requires no table look up and gives a direct solution without iteration. Our approach is guaranteed to provide a solution near or even exactly at the critical point. We demonstrate the usefulness of the approach by implementing our non-iterative phase behavior model into UTCOMP (Chang et al. [17]), a fully compositional model developed at the University of Texas at Austin. Densities and viscosities are calculated within the UTCOMP framework using cubic EOS, and standard mixing rules.

2. New empirical model for flash calculations

In this section we describe our new empirical method for flash calculations of ternary systems. We first consider flash calculations for two-phase systems, and then briefly explain how three-phase regions are treated.

2.1. Two-phase region

Our approach is based on the idea of transforming a ternary system where tie lines in the two-phase region become parallel in the transformed compositional space. Instead of using a constant transformation factor as suggested by Hand, we use a transformation factor that changes with composition.

Fig. 1 illustrates the transformation, where there is a one-to-one mapping of a fixed overall composition to the new overall composition in the transformed space. A given composition z_i in a ternary system is transformed using a transformation factor α so that

$$z_1' = \alpha z_1, \quad z_2' = z_2 \quad \text{and} \quad z_3' = z_3. \tag{1}$$

The transformation factor in Eq. (1) is applied to the lightest component present, although it could also be applied to the heaviest component with the same results. Normalization of the transformed compositions so that they sum to 1.0 gives

$$z_1^* = \frac{z_1'}{z_1' + z_2' + z_3'} = \frac{\alpha z_1}{\alpha z_1 + z_2 + z_3} = \frac{\alpha z_1}{(\alpha - 1)z_1 + 1} \tag{2}$$

and

$$z_2^* = \frac{z_2}{(\alpha - 1)z_1 + 1}, \quad z_3^* = \frac{z_3}{(\alpha - 1)z_1 + 1}. \tag{3}$$

We can easily transform back to the actual composition space if we know α and the transformed composition using

$$z_1 = \frac{z_1^*}{\alpha - (\alpha - 1)z_1^*},$$

$$z_2 = [(\alpha - 1)z_1 + 1]z_2^*, \quad z_3 = [(\alpha - 1)z_1 + 1]z_3^*. \tag{4}$$

Tie lines can also be transformed in the same way because they are a line connected by two equilibrium compositions (x_i, y_i), each of which can be transformed. The only difference is that the transformation factor is determined such that all tie lines become parallel to each other, and to the base tie line in the transformed ternary diagram. The base tie line in Fig. 1 is the 1–3 axis.

These transformation factors are dependent on compositions; each tie line has a different value of α. In the transformed space, this