



Stability analysis for multicomponent mixtures including capillary pressure



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ABSTRACT

Despite the large potential of unconventional resources, many unknowns still exist regarding the physics controlling the extraction processes in these settings. These include accurate representation of phase equilibrium in tight formations and effective implementation of relevant models in simulation tools.

When a fluid is confined in pore spaces of nanometer size, significant interfacial curvatures may occur that can result in large capillary pressures between the liquid and vapor phases: The pressure difference between the two phases will likely affect the vapor-liquid equilibrium state. Previous efforts have shown that this effect is negligible for conventional reservoirs (with pores in the micron range) and current commercial reservoir simulators commonly ignore the effect of capillary pressure in the VLE calculations. However, experimental and modeling efforts have shown that ignoring capillary pressure in the VLE calculations will not be a valid approximation for unconventional (tight) reservoirs.

In this work, we analyze the numerical aspects of including capillarity phenomena in VLE calculations in an effort to arrive at robust and efficient algorithms for stability analysis that can be used in compositional modeling/simulation of unconventional reservoirs. While the equality of chemical potentials is a necessary condition for equilibrium, it is not a sufficient one. A sufficient condition for equilibrium is the minimization of Gibbs energy, and the latter can be tested using the tangent plane distance (*TPD*) criteria. We show that stability analysis based on the *TPD* criteria remains valid for systems with large capillary pressures and propose effective/robust algorithms for stability testing. The proposed algorithms are tested for multicomponent reservoir fluid systems over a range of relevant temperatures, pressures and pore radii.

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1. Introduction

Recent advances in drilling/completion technology have enabled hydrocarbon extraction from tight unconventional resources such as shale gas, liquid-rich shales and tight oil systems. These resources currently contribute significantly to the total oil and gas production in the US. Hydrocarbon in organic-rich shales is one of the most significant unconventional resources [1]. Despite the large potential and the advancement in production technology for these resources, gaps still exist between the physical models used in currently available simulation tools and the well-documented additional complexity of fluid flow and mass transfer in micro- and meso-porous materials. A central challenge is related to the understanding and modeling of phase equilibrium in

confined spaces, e.g. in pores at the nanometer scale, and to develop appropriate and accurate tools/algorithms to be used for estimation of reserves and for forecasting of production [2]. Conventional experimental PVT analysis is usually performed based on the assumption that the porous medium does not influence the phase behavior [3]. However, fluid properties and VLE behavior in confined spaces depart substantially from the corresponding bulk measurements (PVT cell) where vapor-liquid interface curvature can be neglected [4].

When the fluid is confined in small pores, significant interfacial curvatures can arise that results in large a capillary pressure between the equilibrium liquid and vapor phases: A pressure difference that is known to impact the VLE. It has, however, been demonstrated previously that this effect is negligible for conventional reservoirs with pore spaces in the micron range [5,6].

Current commercial reservoir simulators commonly ignore the effect of capillary pressure in VLE calculations. However, experimental and modeling work presented over the past few years

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[3,4,7–10] have shown that neglecting capillary pressure in VLE calculations is not a good assumption for unconventional reservoirs. Furthermore, a standard and reliable measurement of fluid properties and VLE for confined fluids in ultra-tight rocks is still not available [3].

Numerous researchers have worked on analyzing phase envelopes of confined fluids. Nojabaei et al. [8] coupled capillary pressure and phase equilibrium calculations for binary and multicomponent mixtures in confined pores and integrated their model into a compositional reservoir simulator. Based on example calculations, they conclude that better estimates of the producing gas-oil ratio (GOR) are achieved when the capillary pressure is included in the equilibrium calculations. Du and Chu [3] proposed a thermodynamic model to calculate the confined PVT properties for Bakken crude oil systems considering the effects of capillarity in the porous medium. Wang et al. [4] evaluated the effect of capillarity on VLE calculations using a Leverett J-function approach to approximate a saturation dependent capillary pressure. Alharthy et al. [11] proposed a correlation to shift of the phase envelope depending on pore sizes, dividing the pore space into macro-, meso- and micro-porosity, while Sandoval et al. [2] proposed a new algorithm to calculate phase envelopes including the effect of capillary pressure.

Despite a substantial amount of research on the topic of phase behavior of confined fluids, the effect of capillarity in stability analysis has not been extensively studied/documentated to the best of our knowledge. In this work, we will start from Gibbs energy and the requirement for phase stability and introduce modifications needed to account for capillarity in stability analysis. We propose four algorithms for stability testing: Two based on direct/accelerated substitution and two based on minimization. The convergence behavior of the proposed algorithms is illustrated for a range of relevant fluid systems and proximity to critical points. The stability testing is demonstrated to be consistent with the phase boundaries predicted by phase envelope calculations including capillarity. Accordingly, the proposed algorithms provide for reliable tools to study the effect of capillary pressure on phase stability over a wide range of compositions and capillary radii as needed in compositional simulation of unconventional reservoirs/formations.

2. Methodology

In this section, we discuss the stability analysis of a confined fluid and the related impact of capillary pressure. Starting from Helmholtz energy, one can derive the equilibrium condition, in terms of the chemical potential, μ , for a system that includes the contribution from surface energy [12].

$$\mu_i^l(T, p^x, \mathbf{x}) = \mu_i^v(T, p^y, \mathbf{y}), \quad i = 1, \dots, n_c, \quad (1)$$

In Eq. (1), the phase pressures (p^l and p^v) are related through the Young-Laplace equation (written for a spherical interface)

$$p^v - p^l = \frac{2\sigma}{R}. \quad (2)$$

The interfacial tension, σ , is a given function of phase compositions (\mathbf{x} and \mathbf{y}), temperature, T , phase pressures and the radius of curvature of the interface, R . In a capillary tube (pore) the capillary pressure, P_c , is evaluated from

$$P_c = p^v - p^l = \frac{2\sigma \cos \theta}{r_c}, \quad (3)$$

where r_c is pore radius and θ is the contact angle as measured through the denser phase. Although porous rocks are made up by complex networks of non-cylindrical pores of variable radii, we use here a single value (average) representation of the pore radius for

simplicity. We also assume, by default, that the rock is strongly liquid wet ($\theta = 0$). We use the correlation of Macleod [13] and Sugden [14] to calculate interfacial tension (IFT),

$$\sigma = \left[\sum_{i=1}^{n_c} \chi_i (x_i \rho^L - y_i \rho^V) \right]^E, \quad (4)$$

where ρ^L and ρ^V are phase molar densities, x_i and y_i are phase compositions, χ_i is the component parachor and E is an (adjustable) exponent. Researchers have suggested a variety of values for the exponent E . Weinaug and Katz [15] suggested that $E = 4$, while Hough-Stegemeier [16] modified the exponent to $E = 3.66$ for low IFT systems. In 1984, Lee and Chien [17] suggested a value of $E = 3.91$ using critical scaling theory of IFT to evaluate the dependency on temperature. Danesh et al. [18] presented a density-dependent model for exponent E . Schechter and Guo [19] recommended $E = 3.88$ based on experimental data for hydrocarbon systems. In this work, we use $E = 4$ (following Weinaug and Katz). From Eq. (4), one can calculate the interfacial tension, and hence the capillary pressure, for a given set of phase compositions and densities (pressures) of liquid and vapor phases given a pore radius and a contact angle. This allows for a simple algorithm to update the phase pressures by direct substitution as discussed in more detail later.

2.1. Formulation of the stability analysis problem

The tangent plane distance (TPD) of Gibbs has been used repeatedly in developing algorithms for stability analysis of unconfined fluids [20]. To apply this idea for confined fluids, we make the assumption that the volume (or mass) contribution to changes in Gibbs free energy is larger than the interface contribution. In terms of nucleation theory, this is equivalent to assuming that the volume (radius) of any trial phase exceeds the radius of a critical nucleus. Based on this assumption, we can write the TPD at isothermal conditions in the following form

$$TPD(\mathbf{w}) = \sum_{i=1}^{n_c} w_i (\mu_i^w(\mathbf{w}, p^w) - \mu_i^z(\mathbf{z}, p^z)), \quad (5)$$

where \mathbf{z} is the feed composition existing at pressure p^z and \mathbf{w} is a trial phase composition existing at p^w . The assumption of neglecting the interfacial contribution to changes in Gibbs energy, as outlined above, is consistent with the formulation of Sandoval et al. [2] for tracing phase boundaries. This is seen from Eq. (5) where the TPD will equal zero on the phase boundary where the incipient phase (\mathbf{w}) exists in equilibrium with the bulk phase (\mathbf{z}).

At this stage, we can follow the approach of Michelsen [20], and introduce a modified TPD via the variable transformation

$$\ln W_i = \ln w_i - k, \quad (6)$$

where k is the reduced TPD at the stationary points of Eq. (5). The modified reduced TPD , tm , for a system including capillary pressure can then be written in terms of fugacity coefficients

$$tm(\mathbf{W}) = 1 + \sum_{i=1}^{N_c} W_i (\ln W_i + \ln \hat{\varphi}_i^w + \ln p^w - d_i - 1), \quad (7)$$

with

$$d_i = \ln z_i + \ln \hat{\varphi}_i^z + \ln p^z, \quad i = 1, \dots, N_c \quad (8)$$

and

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