A new robust stability algorithm for three phase flash calculations in presence of water

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ABSTRACT

Thermodynamic phase equilibrium calculations for systems containing water are inseparable parts of the compositional hydrocarbon reservoir simulation. In this regard, stability analysis of the phases for distinguishing the existing ones at specific pressures and temperatures is a principal part of such calculations. This study is aimed to develop a new stability algorithm with application to three phase flash calculations in the presence of brine. The developed scheme is capable of doing the phase behavior calculations in a more robust way compared to the other available algorithms. Henry's law is utilized to predict the aqueous phase properties, and a new initial guess is provided for three phase flash calculations that assures the convergence of the scheme. It is shown that the proposed procedure is able to handle the systems with high CO_2 content while the available schemes in the literature fail.

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1. Introduction

Hydrocarbon reservoirs are explored mostly in sandstone or carbonate rocks. These rock types were originally formed in aquatic environments, and they were saturated with water before secondary migration. In secondary migration, oil comes through the reservoir rock from the source rock and displaces water (Tissot and Welte, 2013). Water-wet nature of reservoir rocks causes incomplete displacement of water by immigrated oil. As a result, water remains in hydrocarbon reservoirs in the form of a thin layer covering the rock grains or as a trapped phase in small pores and throats. This water saturation is called as connate water saturation (Anderson, 1987a, 1987b).
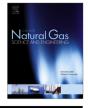
Water may also be present below the hydrocarbon reservoir in the form of an aquifer. In this case, water will invade the reservoir rock after pressure decline (Ahmed, 2006). In addition to the so-called sources of water in hydrocarbon reservoirs, water may also be injected into the reservoir with the purpose of enhancing oil recovery (Willhite, 1986; Green and Willhite, 1998). According to the aforementioned reasons, water is an inseparable component of reservoir fluids and ignoring water in petroleum reservoir fluid phase calculations, has inappropriate consequences like inaccurate or even inconsistent results of reservoir simulation. It is worthy to mention that there is no pure water in the reservoir, so taking account of dissolved salts and ions are crucial factors which can affect the behavior of reservoir fluid, since it has a strong effect on gas solubility in the aqueous phase (Li and Nghiem, 1986).

Various equations of states (EOS) are used in the petroleum industry for the purpose of modeling petroleum fluid phase behavior (Avlonitis et al., 1994). The most widely used types are cubic EOS like RK (Redlich and Kwong, 1949), SRK (Soave, 1972) and Peng-Robinson (Peng and Robinson, 1976). In the case of reservoir fluids, vapor and liquid hydrocarbon phases are modeled with these EOS in a range of reasonable error, while the predicted behavior of aqueous phase by these EOS is not yet acceptable. Several researchers have made effort to model water-rich (aqueous) phase with the same EOS as vapor and liquid hydrocarbon phases (Heidemann, 1974; Evelein et al., 1976; Peng and Robinson, 1980; Mokhatab, 2003). They found that accurate prediction of aqueous phase behavior is difficult to achieve with the original form of EOS, so they made some modifications in that EOS in order to achieve a higher degree of accuracy in results (Erbar, 1980; Peng and Robinson, 1980; Reshadi et al., 2011).

On the other hand, various researchers discarded using EOS for water-rich phase and used other thermodynamic approaches like Henry's law for modeling the aqueous phase behavior and an EOS

for liquid and vapor hydrocarbon phases (Luks et al., 1976; Mehra et al., 1982; Nghiem and Heidemann, 1982; Li and Nghiem, 1986; Carroll and Mather, 1997). Since hydrocarbon components are sparingly soluble in the aqueous phase, Henry's law constraint is satisfied in the case of three phase flash calculation in the presence of water. Moreover, comparison of results with experimental data shows a good prediction of aqueous phase behavior using Henry's law (Mackay et al., 1979; Li and Nghiem, 1986; Altschuh et al., 1999).

Nghiem and Heidemann (1982) performed three phase hydrocarbon-brine flash calculation using Henry's law for modeling of water-rich phase. Since there were not any safely generalized correlations for Henry's law constants until that time, they used Henry's constants calculated from experimental data and only considered the solution of carbon dioxide component in water. They also neglected the presence of water in vapor and liquid hydrocarbon-rich phases. Li and Nghiem (1986) proposed a correlation for calculation of Henry's constants with respect to pressure and temperature for various hydrocarbon components of petroleum industry interest. They also considered the effect of brine salinity, using the scaled-particle theory (SPT) to modify Henry's law constants derived for pure water.

Lapene et al. (2010) introduced a new three-phase free-water flash method by using modified Rachford-Rice equation. Their proposed algorithm guarantees the convergence of flash calculations. They assumed water as a free phase and neglected the dissolution of hydrocarbon components in aqueous phase. However, they took the water coexistence with hydrocarbon in vapor and liquid hydrocarbon rich phases into consideration. Their algorithm also does not consider the disappearance of water-rich phase, which can happen in low water-content feeds at high temperature or low-pressure ranges.

In addition to EOS selection and phase behavior prediction of reservoir fluid in the flash calculation, phase stability analysis is another important issue in this realm. By means of phase stability analysis, one can predict the presence of phases at a certain pressure and temperature. For instance, there may exist only a hydrocarbon-rich vapor phase in a high temperature and low pressure for a low-water-content overall composition (feed). Two main approaches have been introduced to solve the phase stability problem: the stationary points method (classical method) and the direct minimization of the tangent plane distance (TPD) function (Nichita et al., 2002).

The stationary points method was developed by Michelsen (1982b) and used by many researchers for multicomponent flash calculation phase stability check (Nghiem et al., 1983; Li and Nghiem, 1986; Nelson, 1987; Gupta et al., 1991; Ballard and Sloan, 2004; Ghosh et al., 2004). Li and Nghiem (1986) proposed a flow diagram of a stepwise phase stability check procedure for three phase flash calculations in the presence of water. Their stability test method was developed for determining the stable phases at specified pressures and temperatures among liquid, vapor and/or aqueous phases. Their proposed procedure fails to detect the phases, accurately, in some cases that will be discussed in results and discussion part.

In this work, a new stability algorithm is proposed for three phase flash calculation in the presence of water and its validity is checked by means of performing a flash calculation on two different overall compositions. The proposed stability algorithm identifies the stable phases suitably at different pressures and temperatures even for systems with high CO_2 content while other available schemes fail. Additionally, a new general initial guess is provided for three phase flash calculation which guarantees the convergence of the calculations under different situations.

2. Theory

2.1. Henry's law

As discussed earlier, vapor and liquid phases are modeled using any adequate EOS, but, the water-rich phase is modeled using Henry's law. The reason behind using Henry's law for this phase is that the solubility of hydrocarbon components in water is low (Polak and Lu, 1973; Wasik and Brown, 1973; Li and Nghiem, 1986). Henry's law constant for a sparingly soluble component in water is defined as follows:

$$HLC = \frac{Partial\ pressure\ in\ gas\ phase}{Mole\ fraction\ in\ aqueous\ phase} \tag{1}$$

Equation (1) can also be expressed in terms of fugacity that is handy in flash calculations:

$$f_{i\ aq} = y_{i\ aq} H_i \quad i \neq w \tag{2}$$

Subscripts aq and w denote aqueous phase and water component, respectively. H_i is the Henry's law constant of component i in the aqueous phase. Smith et al. (2001) proposed a differential equation for calculating changes of Henry's law constant with respect to pressure and temperature, as follows:

$$d(\ln(H_i)) = \frac{V_{m\ i}^{\infty}}{RT} dP + \frac{h_{i\ v} - h_i^{\infty}}{RT^2} dT \tag{3}$$

where $V_{m\ i}^{\infty}$ is partial molar volume of component i in the aqueous phase at infinite dilution, $h_{i\ v}$ is the enthalpy of component i in the vapor phase, and h_i^{∞} is the enthalpy of component i in the aqueous phase at infinite dilution. The term $h_{i\ v} - h_i^{\infty}$ is strongly dependent on temperature but there is not any available correlation for describing its dependency. It has also been found that, $V_{m\ i}^{\infty}$ is usually not very sensitive to pressure (Li and Nghiem, 1986). Therefore, for a given temperature, integration of equation (3) from P^0 to P gives:

$$\ln(H_i) = \ln\left(H_i^0\right) + \frac{V_{m\ i}^{\infty}\left(P - P_i^0\right)}{RT} \tag{4}$$

where H_i^0 is henry's law constant at reference pressure P_i^0. Equation (4) can also be written as:

$$\ln(H_i) = \ln\left(H_i^*\right) + \frac{V_i^{\infty} P}{RT} \tag{5}$$

where H_i^* is defined as below:

$$\ln\left(H_i^*\right) = \ln\left(H_i^0\right) - \frac{V_{m\ i}^{\infty} P_i^0}{RT} \tag{6}$$

In this study, Equation (6) is used for calculating Henry's law constant from solubility data and H_i^* is defined as the reference Henry's law constant. The molar volume at infinite dilution is calculated using the following correlation proposed by Lyckman et al. (1965):

$$\frac{P_{c\ i} V_{m\ i}^{\infty}}{RT_{c\ i}} = 0.095 + 2.35\left(\frac{TP_{c\ i}}{CT_{c\ i}}\right) \tag{7}$$

where C is the cohesive energy density of water given by: