



Three-phase free-water flash calculations using a new Modified Rachford–Rice equation

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ABSTRACT

A novel Modified Rachford–Rice equation is developed for three-phase equilibrium calculations in hydrocarbon–water systems, based on the free-water assumption, i.e., the water-rich liquid phase consists of pure water only. In the inner loop of the flash algorithm, the three-phase problem (consisting in a system of two non-linear equations) is replaced by a pseudo-two-phase problem (consisting in a non-linear equation). Unlike previous formulations, the new Modified Rachford–Rice function is guaranteed to monotonically decrease between two adjacent asymptotes. The negative flash concept is used, and a search window is proposed for the vapor fraction. The new free-water flash method proved to be robust, and excellent agreement between full three-phase flash and pseudo-two-phase free-water flash was obtained for various test problems. The proposed method is very useful in compositional reservoir simulation of certain oil recovery methods and in process simulation.

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1. Introduction

Processes involving hydrocarbon mixtures and water are commonly encountered in petroleum industry, either in downstream (refinery and oil and gas processing) or upstream (reservoir) simulations. A considerable number of phase equilibrium calculations may be required in compositional reservoir simulation or in real-time dynamic process simulations; even if only two-phase calculations are involved, computational time associated with thermodynamic calculations can account for most of the total CPU time. The picture become more complicated when multiphase equilibrium calculation have to be performed, since some problems such as initialization (which usually require phase stability testing), phase appearance/disappearance during iterations, or phase assignment are more complex (or specific) in a multiphase context. Robustness is essential, since a failure during a simulation run is fatal.

Three-phase equilibrium calculations for water–hydrocarbon mixtures are required in compositional reservoir simulation of some thermal recovery methods, such as steam injection, in situ combustion, or for CO₂ sequestration modeling.

The most common way was to perform a two-phase equilibrium calculation combined with a steam table instead of a real three-phase equilibrium calculation [1–3]. Basically, equilibrium calculation is performed first without water in order to get phase repartition and compositions for the hydrocarbon-rich phase and the vapor phase, then water is taken into account using a steam table; this approach is fast but not consistent, since adding water breaks equilibrium and may results in over or under estimation of evaporation or condensation. The development of compositional thermal simulators in conjunction with equation of state formulations (which are fully consistent) has received an increasing attention in the recent years [1,4–7]. Such formulations require three-phase flash calculations in each gridblock at each time step.

If equilibrium constants are taken as primary variables, multiphase flash calculations consist in finding the phase distribution (solving the Rachford–Rice equations) in an inner loop and updating the equilibrium constants in an outer loop. Phase distribution can be calculated either by solving a minimization problem [8,9], or by solving a non-linear system of equations [10]. Note that resolution of Rachford–Rice equations can be avoided only in second-order methods with component mole numbers [11] or reduction parameters [12] as iteration variables.

For hydrocarbon–water systems, efficient formulations can be obtained by mapping the three-phase flash to a pseudo-two-phase flash; this is possible if repartition of water between the two phases (vapor and hydrocarbon-rich) can be predetermined in some way [13]. In this case, the resolution of a non-linear system of equa-

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tions (their number is the number of phases minus one) in the flash inner loop is replaced by the resolution of a non-linear equation. This is the idea behind the so-called “free-water” flash approach. The free-water assumption means that the solubility of hydrocarbon components in the water-rich liquid phase is neglected, that is, this phase consists of pure water. The free-water assumption is supported by the fact that the solubility of hydrocarbon (typically of the order of 10^{-4}) in the water-rich phase is several orders of magnitude smaller than the solubility of water (typically of the order of 10^{-2}) in the hydrocarbon-rich phase. Tang and Saha [13] presented an interesting free-water flash method. They proposed a new Modified Rachford–Rice (MRR) equation and a quick-phase determination approach based on Nelson criteria [14]. However, their MRR equation is not monotonic and its resolution is very difficult in some particular cases.

Recently, Iranshahr et al. [5] presented a free-water flash method designed for thermal compositional simulation. The method admits an additional assumption, i.e., the solubility of water in the hydrocarbon-rich liquid phase is neglected. Moreover, the objective function is not guaranteed to be monotonic (thus Newton methods cannot be used for solving the MRR equation).

The goal of this work is to propose a new three-phase free-water flash method especially fitted for reservoir thermal compositional simulation. A novel Modified Rachford–Rice equation is developed, with a monotonic objective function, and the negative flash concept [15] is used. The proposed method is tested for several representative examples and proved to be robust and accurate. Comparison of free-water flash results with full three-phase flash results show that the free-water assumption does not induce significant deviations from the “true” equilibrium.

2. Modified Rachford–Rice equation

2.1. Derivation of the MRR equation

Equilibrium of each species in the three-phase case is expressed as:

$$f_i^O = f_i^V = f_i^W; \quad i = 1, nc \quad (1)$$

and using fugacity coefficients as:

$$P\phi_i^O x_i^O = P\phi_i^V y_i = P\phi_i^W x_i^W; \quad i = 1, nc \quad (2)$$

The two equilibrium ratios are defined as:

$$K_i^I = \frac{y_i}{x_i^O} = \frac{\phi_i^O}{\phi_i^V}; \quad i = 1, nc \quad (3)$$

$$K_i^{II} = \frac{y_i}{x_i^W} = \frac{\phi_i^W}{\phi_i^V}; \quad i = 1, nc \quad (4)$$

In a free-water system, water is distributed over the three phases whereas all other components are present only in vapor and hydrocarbon (non-aqueous) phases. This assumption reads

$$x_{i=w}^W = 1; \quad x_{i \neq w}^W = 0 \quad (5)$$

Thus, Eq. (4) is simplified for the water component and takes the following form

$$y_w = K_w^{II} \quad (6)$$

and from Eq. (3):

$$x_w^O = K_w^{II}/K_w^I \quad (7)$$

In the rest of this paper, we use the notations $K_i^I = K_i$ and $x_w^O = x_w$.

The component material balance equation for VOW systems is

$$z_i = y_i V + x_i^O O + x_i^W W; \quad i = 1, nc \quad (8)$$

and the overall material balance equation is

$$V + O + W = 1 \quad (9)$$

Using Eqs. (6)–(8) for the water component, an expression for the water fraction is obtained

$$W = \frac{z_w + V(x_w - y_w) - x_w}{1 - x_w} \quad (10)$$

For non-water components, Eq. (8) can be written as following, using Eqs. (3) and (9)

$$z_i = x_i^O K_i V + x_i^O (1 - V - W); \quad i \neq w \quad (11)$$

Finally, using Eq. (10), expressions of the mole fractions of component i in hydrocarbon-rich liquid and vapor phases as functions of feed composition, equilibrium constants and vapor fraction are obtained from Eq. (11)

$$x_i^O = \frac{z_i}{1 + V(K_i - 1) - W} = \frac{z_i}{1 + V(K_i - 1 + \frac{y_w - x_w}{1 - x_w}) + \frac{x_w - z_w}{1 - x_w}}; \quad i \neq w \quad (12)$$

$$y_i = x_i^O K_i = \frac{z_i K_i}{1 + V(K_i - 1 + \frac{y_w - x_w}{1 - x_w}) + \frac{x_w - z_w}{1 - x_w}}; \quad i \neq w \quad (13)$$

The challenge now, is to find a Modified Rachford–Rice equation that is monotonic between adjacent asymptotes. The new constraint function is constructed starting from the original Rachford–Rice equation

$$F(V) = \sum_{i=1}^{nc} (y_i - x_i^O) = 0 \quad (14)$$

by adding the term $\frac{y_w - x_w}{1 - x_w}$ to both sides of Eq. (14)

$$\sum_{i=1}^{nc} \left[y_i - x_i^O + x_i^O \left(\frac{y_w - x_w}{1 - x_w} \right) \right] = \frac{y_w - x_w}{1 - x_w} \quad (15)$$

Then, if water terms are removed from summation, Eq. (15) becomes

$$\sum_{i \neq w}^{nc} \left[y_i - x_i^O + x_i^O \left(\frac{y_w - x_w}{1 - x_w} \right) \right] + x_w - y_w + x_w \left(\frac{y_w - x_w}{1 - x_w} \right) = \frac{y_w - x_w}{1 - x_w} \quad (16)$$

or, after elementary algebraic operations

$$\sum_{i \neq w}^{nc} \left[y_i - x_i^O + x_i^O \left(\frac{y_w - x_w}{1 - x_w} \right) \right] = 0 \quad (17)$$

This last relation can be extended using Eqs. (12) and (13) as

$$G(V) = \sum_{i \neq w}^{nc} \frac{z_i (K_i - 1 + \frac{y_w - x_w}{1 - x_w})}{1 + V(K_i - 1 + \frac{y_w - x_w}{1 - x_w}) + \frac{x_w - z_w}{1 - x_w}} = 0 \quad (18)$$

or further

$$G(V) = \sum_{i \neq w}^{nc} \frac{z_i (K_i - K_w^*)}{V(K_i - K_w^*) + K_w^z} = 0 \quad (19)$$

where the notations

$$K_w^* = \frac{1 - y_w}{1 - x_w} \quad (20)$$

and

$$K_w^z = \frac{1 - z_w}{1 - x_w} \quad (21)$$

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