Fluid Phase Equilibria 267 (2008) 6–17

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

A robust negative flash based on a parameterization of the tie-line field

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ARTICLE INFO

Article history:
Received 5 December 2007
Received in revised form 30 January 2008
Accepted 12 February 2008
Available online 19 February 2008

Keywords:
Phase behavior
Flash
Negative flash
Tie line
K-value
Ternary diagram
Quaternary diagram
Quadratic curve
Quadric surface

ABSTRACT

We propose a novel approach to flash calculation, with particular application to negative flash. The basis of the method is a parameterization of the tie-line field. Rather than solving the Rachford–Rice equation (or any of its variants) we solve directly for the parameters defining the tie line. For an N-component system, our approach leads to a system of $N-2$ *quadratic* equations, which we solve efficiently using a Newton method. The iterative method is very robust: unlike other negative flash procedures, the solution displays continuous dependence on the overall composition, even in the transition to negative concentrations. We illustrate the properties and behavior of the proposed approach on three-component and four-component systems, and we then generalize the method to systems of N components. From the global triangular structure of the system with constant K-values, it follows that the system of N^{-2} quadratic equations can only have two roots. For the important case of three components, the flash calculation is explicit.

1. Introduction

A flash calculation consists in determining the amount of gas and liquid (and their composition) of a mixture with a known overall composition. It is an integral part of computational models in both the upstream and downstream oil industry. Flash calculations can be responsible for a significant fraction of the computational time in compositional reservoir simulation models [1].

At equilibrium, a two-phase mixture will satisfy

$$K_i = \frac{y_i}{x_i}, \tag{1}$$

for all of its chemical components $i = 1, \dots, N$. In Eq. (1), y_i and x_i are the mass fraction of component i in the vapor and liquid phases, respectively, and K_i is the equilibrium ratio (also known as K-value) for that component. In general, the K-values depend on pressure, temperature and overall composition. In this paper, we shall assume that K-values are constant. This is often a good approximation for many hydrocarbon systems at moderate pressures and temperatures [13]. When this is not the case, the methodology presented here must be understood as the building block for an overall flash calculation in which an outer iteration is performed to determine the K-values [12,13,20,21].

The flash problem can be expressed as follows: given a set of positive K-values, K_i, and non-negative overall concentrations C_i satisfying $\sum_{j=1}^{N} C_j = 1$, find the gas saturation S and the concentrations in the liquid and vapor, x_i and y_i, respectively, such that

$$C_i = (1-S)x_i + S y_i \quad \text{for all } i = 1, \dots, N \tag{2}$$

with the restrictions

$$\sum_{j=1}^{N} x_j = 1, \quad \sum_{j=1}^{N} y_j = 1, \quad y_i = K_i x_i \quad \text{for all } i = 1, \dots, N. \tag{3}$$

The standard procedure for solving the flash problem is to note that

$$\sum_{j=1}^{N} y_j - \sum_{j=1}^{N} x_j = 0. \tag{4}$$

Several variants of this equation exist. The original method proposed by Rachford and Rice [14] expressed it as a function of the vapor saturation S. Whitson and Michelsen [21] showed that this procedure will converge even if the mixture is in the single-phase region (a calculation known as negative flash), as long as

$$\frac{1}{1-K_{\max}} < S < \frac{1}{1-K_{\min}}. \tag{5}$$

If the overall composition is far away from the two-phase region – in particular, if it is outside the region of positive overall com-

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doi:10.1016/j.fluid.2008.02.009

positions – Wang [18], and Wang and Orr [20], proposed to solve Eq. (4) in terms of a liquid composition x_l for some component $l \in \{1, \ldots, N\}$—in fact, they assumed that $l \equiv 1$ in all cases. As we show in the next section, this procedure may diverge or converge to a spurious root even if the initial guess is arbitrarily close to the root.

The ability to compute a negative flash for *any* composition state is important in practice. The construction of analytical solutions for multicomponent systems relies heavily on the identification of tie lines (for states in the two-phase region) and tie-line extensions (for states in the single-phase regions) [2,4–8,13,15,17,19]. Analytical solutions to oil/gas displacements by the method of characteristics are at the heart of some techniques for the calculation of the minimum miscibility pressure [3,20], and are the key building blocks for fast simulation of multidimensional reservoir flows by the front-tracking/streamline method [9,10,16].

A tie line is a straight line in composition space that connects a liquid composition to a gas composition, both states being at thermodynamic equilibrium. Therefore, the flash problem is solved if, for a given overall composition state, the tie line passing through that state is identified. Jessen et al. [3] presented an approach to the calculation of minimum miscibility pressure in which tie-line intersections were computed using a novel co-linearity condition that avoided convergence problems of the negative flash approaches of Refs. [21,20]. It is in this context – tie line identification in the single-phase region through a negative flash – that the developments presented here are relevant.

We propose a new approach for the (negative) flash problem. In Section 2, we use the three-component system to illustrate the shortcomings of existing negative flash procedures, and to develop the rationale for the new method. In this important case, the flash problem reduces to the solution of a quadratic equation. We extend our analysis to the four-component system in Section 3, where we show that our parameterization of the tie-line field leads to a system of two *quadratic* equations. We provide a geometric interpretation of the solution as the intersection of two conics. Newton iteration leads to quadratic convergence to the physical solution in all cases. In Section 4 we generalize the framework to the N-component system. In Section 5 we give some concluding remarks.

2. Three-component system

Without loss of generality, we shall assume that the K-values satisfy the following ordering relations:

$$K_1 > K_2 > K_3, \quad K_1 > 1, \quad K_3 < 1. \tag{6}$$

Two cases are possible: a high-volatility intermediate component ($K_2 > 1$), and a low-volatility intermediate component ($K_2 < 1$). Typical phase diagrams for these two cases are shown in Figs. 1 and 2, respectively. Compositions close to the C_1-vertex are in vapor phase, and compositions close the C_3-vertex (the origin) are in liquid phase. For constant K-values, the vapor and liquid loci (the curves separating the single-phase regions from the two-phase region) are straight lines. We denote by $\hat{\boldsymbol{x}}_i$ and $\hat{\boldsymbol{y}}_i$ the intersections of the liquid and gas loci, respectively, with the C_i-axis:

$$\hat{\boldsymbol{x}}_1 = \begin{bmatrix} \hat{x}_1 \\ 0 \end{bmatrix}, \quad \hat{x}_1 = \frac{1 - K_3}{K_1 - K_3}, \qquad \hat{\boldsymbol{y}}_1 = \begin{bmatrix} \hat{y}_1 \\ 0 \end{bmatrix}, \quad \hat{y}_1 = K_1 \frac{1 - K_3}{K_1 - K_3}, \tag{7}$$

$$\hat{\boldsymbol{x}}_2 = \begin{bmatrix} 0 \\ \hat{x}_2 \end{bmatrix}, \quad \hat{x}_2 = \frac{1 - K_3}{K_2 - K_3}, \qquad \hat{\boldsymbol{y}}_2 = \begin{bmatrix} 0 \\ \hat{y}_2 \end{bmatrix}, \quad \hat{y}_2 = K_2 \frac{1 - K_3}{K_2 - K_3}. \tag{8}$$

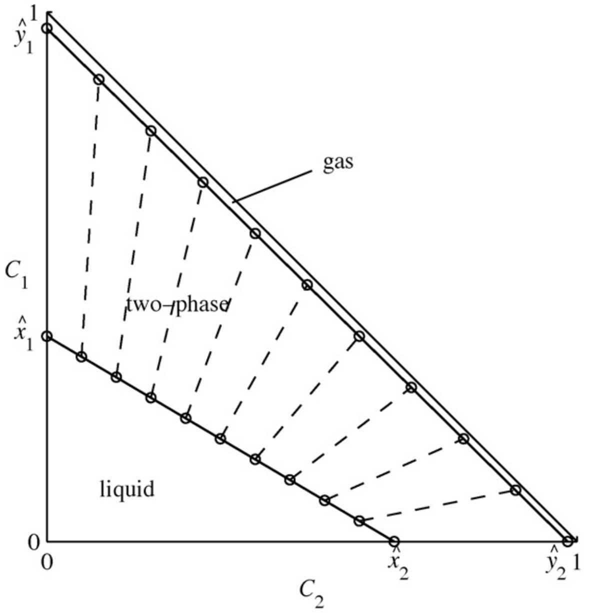

Fig. 1. Ternary diagram and tie-line field for $K_2 > 1$.

If $K_2 > 1$, the C_2-component is a gas and the numeric values of $\hat{x}_2$ and $\hat{y}_2$ are less than 1. In this case, the two-phase region extends to the C_2-axis. In contrast, if $K_2 < 1$, the C_2-component is a liquid and $\hat{x}_2 > \hat{y}_2 > 1$. This means that the liquid and vapor lines intersect the diagonal edge of the triangle corresponding to $C_3 = 0$.

For any composition state on the unit triangle there exist liquid and vapor compositions that are in thermodynamic equilibrium. The straight line connecting such two compositions is called a *tie line*. Figs. 1 and 2 show the tie-line field for the cases $K_2 > 1$ and $K_2 < 1$, respectively.

2.1. Whitson and Michelsen negative flash

Combining Eqs. (1) and (4), the Rachford–Rice equation may be written in the following residual form as a function of gas saturation:

$$R(S) = \sum_{j=1}^{N} \frac{(K_j - 1)C_j}{1 + (K_j - 1)S} = 0. \tag{9}$$

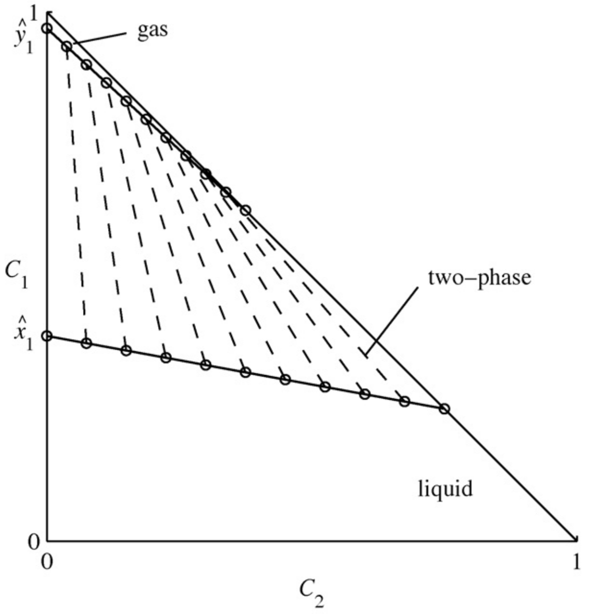

Fig. 2. Ternary diagram and tie-line field for $K_2 < 1$.