



## A rapid and robust alternative to Rachford–Rice in flash calculations

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### ABSTRACT

Rachford–Rice iterations are widely used in equation-of-state (EOS) flash calculations to determine phase equilibrium compositions from constant equilibrium ratios ( $K$ -values). The method, however, can be slow to converge or may not converge at all for cases where at least one overall composition is zero or negative. Having a robust method for flash calculations in these special cases is important in calculating the minimum miscibility pressure (MMP) using method of characteristics (MOC).

This paper presents a simple, fast, and robust alternative to Rachford–Rice and similar methods in flash calculations, whether overall compositions are positive, zero, or negative. The new objective function has two fewer asymptotes compared to Rachford–Rice and is based on solving for one of the equilibrium phase mole fractions, typically the lightest component.

Results with the new objective function demonstrate that rapid convergence using Newton–Raphson (NR) iterations is assured because the correct solution is determined within a small range (window). In that window, no poles exist no matter the overall composition and the objective function is often nearly linear. Improved linearity of the objective function contributes to increased convergence speed even near critical points.

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### 1. Introduction

Compositional simulation is often required to model the complex interaction of flow with phase behavior when gas is injected into oil reservoirs. This is especially true for miscible or nearly miscible floods where black-oil simulation is not accurate.

A significant disadvantage of compositional simulation, however, is that flash calculations with cubic EOS are computational intensive and may not be reliable near critical regions. Research has shown that EOS flash calculations can occupy 50–70% of total computational time in compositional simulations [1]. Repeated flash calculations with cubic EOS are also needed in other problems such as multiphase flow in pipelines [2] and determination of minimum miscible pressure (MMP) or minimum miscible enrichment (MME) from analytical methods [3,4]. Analytical methods for the determination of MMP or MME often require flash calculations in negative composition space or where one overall composition is zero.

There are two approaches to calculate the equilibrium compositions and phase molar fractions from a cubic EOS: (1) direct minimization of the mixture molar Gibbs energy [5–7] or (2) chemical potential equality (in terms of fugacity). The Rachford–Rice method [8] is used extensively as a subroutine in flash calculations in conventional compositional simulation. Rachford and Rice [8] derived a simple objective function assuming constant  $K$ -values to calculate phase compositions for two equilibrium phases. They used an iterative bisection method where the phase molar fraction, either liquid or vapor, is constrained to lie in the range from 0.0 to 1.0. Equilibrium phase compositions are then calculated by mass balance from the converged phase molar fraction and the overall compositions. Their method works well for the overall composition that lies inside the two-phase region. However, their objective function has many poles and roots and is often very nonlinear. Moreover, when the overall composition lies outside the two-phase zone, the correct root is not between 0.0 and 1.0. Li and Nghiem [9] extended the Rachford–Rice method to negative flash calculations, where the overall composition can be outside the two-phase zone so that the solution for phase molar fractions is less than 0.0 or greater than 1.0. They also improved the speed of convergence by using Newton–Raphson (NR) iterations. Because of the

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## Nomenclature

$a$	attraction parameter for EOS (psia ft <sup>3</sup> /lbm mol)
$b$	repulsion parameter for EOS (ft <sup>3</sup> /lb mol)
$\hat{f}$	component fugacities (psia)
$k$	binary interaction parameter (dim.)
$K$	$K$ -value (dim.)
$L$	liquid mole fraction (dim.)
$N_C$	number of components
$N_P$	number of phases
$P$	reservoir pressure (psia)
$R$	gas constant (psia ft <sup>3</sup> /lb-mol R)
$T$	temperature (°F)
$V$	vapor mole fraction (dim.)
$\bar{V}$	molar volume (ft <sup>3</sup> /lb mol)
$x$	liquid phase molar composition (dim.)
$y$	vapor phase molar composition (dim.)
$z$	overall composition (dim.)
$\alpha$	transformation parameter (dim.)
$\hat{\phi}$	component fugacity coefficient (dim.)

### Superscripts and subscripts

*	transformed composition
$i, j$	species index
$j, k$	phase index
$m$	mixture
max	upper boundary of the investigation range
min	lower boundary of the investigation range
ref	reference component

multiplicity of poles and roots, their method could easily diverge from the correct root.

Whitson and Michelsen [10] made a significant improvement in the robustness of the negative flash calculation by specifying a range or window in which the correct root of the phase molar fraction should lie. Furthermore, they showed that there are no poles within that range as long as overall compositions are positive. Because of the nonlinearity of the Rachford–Rice objective function, however, convergence could still be slow. For the special case when one or more overall compositions are negative or zero, the correct root does not lie within their proposed window so that convergence is not guaranteed or in some cases is not even possible.

Several authors [11–14] derived a new objective function by multiplying the Rachford–Rice function by its denominators (poles). This approach makes the new objective function more continuous than the Rachford–Rice objective function. However, the new function is more computationally intensive and nonlinear than the original Rachford–Rice function. Thus, this approach offered no significant advantages over the Rachford–Rice function with the Whitson and Michelsen window.

Leibovici and Neoschil [15] continued this approach, by multiplying the Rachford–Rice objective function by the denominators of the poles corresponding to the lightest and heaviest components. They gave a smaller window for the phase mole fraction than that of Whitson and Michelsen and showed improvement in average computational time for the flash calculations considered. Their method, however, still has problems with nonlinearity of the objective function, especially when the lightest and heaviest components are present in small amounts and the overall composition is close to either the bubble-point or dew-point curves. Their method also suffers from increased computational cost per iteration and in most cases of practical interest will not be faster than Rachford–Rice. Last, their method cannot be extended to equilibrium calculations with more than two phases [16], and is therefore not a general approach.

Wang and Orr [17–19] focused on solving the negative flash problem for overall compositions outside of positive composition space where at least one overall composition is negative (or zero). Their goal was primarily to improve convergence for overall compositions outside of positive composition space for MMP calculations using the method of characteristics. They initially used a system of equations to solve for the liquid phase compositions, instead of phase saturations. This approach, however, is inefficient, because it requires solution of a system of equations and can converge to a root where one or more liquid equilibrium compositions are negative. Wang [19] modified the procedure using only a single function, and solved for only one liquid equilibrium phase composition, the lightest component  $x_1$ . This approach made the calculation faster, and potentially more robust, but it introduced a trivial solution at  $x_1 = 0$ .

Juanes [20,21] recently presented a method derived from Wang and Orr's [18] original set of equations, but where he parameterized the bubble-point curve resulting in a set of  $N_C - 2$  quadratic equations. Similar to Wang and Orr's method, his method is not efficient and could converge to a false tie-line (one with negative equilibrium compositions). An important conclusion of his research, however, is that at most two roots (or two tie lines) exist in the solution domain for the case when overall compositions can be negative. This has important implications to the uniqueness of the method of characteristics solution for the estimation of miscibility pressure in petroleum gas floods (see for example uniqueness questions raised in Yuan and Johns [4]).

In this paper, we derive a new objective function that is often nearly linear in terms of a selected equilibrium liquid phase mole fraction. We then derive a small window in which the physical root(s) must lie. Several example calculations are performed and the results are compared to the Rachford–Rice, Wang and Orr, and Leibovici and Neoschil methods. The Peng–Robinson [22] EOS is also used in example calculations to demonstrate that the function can converge very near the critical region.

## 2. Conventional flash calculation by cubic EOS

For an equilibrium flash calculation, the pressure, temperature, and overall mole fractions are specified and the amounts of the phases and their compositions that form at equilibrium are calculated. An expression for the fugacities of each component in each phase is needed to calculate phase equilibrium. At equilibrium,

$$\hat{f}_i^j = \hat{f}_i^k, \quad i = 1, \dots, N_C; \quad j, k = 1, \dots, N_P \quad (1)$$

where  $\hat{f}_i$  is the fugacity of a component,  $N_P$  is the number of phases, and  $N_C$  is the number of components. For vapor–liquid equilibrium, Eq. (1) can be rewritten in terms of the component fugacity coefficients  $\hat{\phi}_i$  as,

$$x_i P \hat{\phi}_i^L = y_i P \hat{\phi}_i^V, \quad i = 1, \dots, N_C \quad (2)$$

where  $P$  is the reservoir pressure,  $x_i$  is the liquid equilibrium phase composition, and  $y_i$  is the vapor equilibrium phase composition.

The general procedure for a two-phase flash calculation is well-documented in the literature and is outlined briefly in Appendix D.

## 3. Rachford–Rice iterations

Rachford–Rice iterations are typically used to determine the phase compositions and amounts as outlined in Step 3. The objective function for this method is easily derived from the definition of  $K$ -values for two-phase equilibrium:

$$y_i = K_i x_i, \quad i = 1, \dots, N_C \quad (3)$$

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