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Multiphase isenthalpic flash integrated with stability analysis

Di Zhu, Ryosuke Okuno*

University of Texas at Austin, USA

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ABSTRACT

Isobaric, isenthalpic (PH) flash is challenging for multiphase non-isothermal flow simulation using an equation of state (EOS). This is because the number of equilibrium phases is unknown in temperature and composition space, and because the system of equations in PH flash becomes nearly degenerate for narrow-boiling fluids. The term “narrow-boiling” is used in the literature to refer to enthalpy that is sensitive to temperature.

The primary objective of this research is to develop the multiphase PH-flash algorithm integrated with stability analysis that resolves the two technical challenges mentioned above. The secondary objective is to present a new analysis of narrow-boiling behavior by coupling energy and phase behavior equations through the temperature dependency of K values. The thermodynamic model used is the Peng-Robinson EOS with the van der Waals mixing rules.

PH flash in this research is formulated by use of the tangent-plane-distance function, in which phase-split computation is integrated with phase-stability analysis. The formulated PH flash is solved by the direct-substitution algorithm with an arbitrary number of sampling compositions (N_S), at which phase stability is measured during the iteration. The number of equilibrium phases is not required to be fixed in the new algorithm.

Results in case studies show that the new algorithm can robustly handle phase appearance/disappearance with narrow-boiling behavior, including the case of one degree of freedom. The algorithm becomes more robust with increasing N_S because the possibility of finding all stationary points of the tangent-plane-distance function increases. However, the number of iterations required tends to increase with increasing N_S because the algorithm with more sampling compositions may take more iterations for merging and adding some of the sampling compositions.

The general condition presented for narrow-boiling behavior is that the interplay between energy balance and phase behavior is significant. Two subsets of the condition are derived by analyzing the convex function whose gradient vectors consist of the Rachford-Rice equations; (i) the overall composition is near an edge of composition space, and (ii) the solution conditions (temperature, pressure, and overall composition) are near a critical point, including a critical endpoint. A special case of the first specific condition is the fluids with one degree of freedom. These conditions for narrow-boiling behavior are demonstrated in case studies.

1. Introduction

Numerical solution of isothermal compositional reservoir flow has been extensively studied [1–20]. For thermal compositional reservoir flow, however, the literature is relatively scarce [21–31]. Reliable solution of the coupled equations of mass balance, energy balance, and phase behavior requires a detailed understanding of numerical difficulties that may occur in thermal compositional simulation. This paper is concerned with two major issues in isenthalpic flash for thermal compositional simulation with a cubic equation of state (EOS); one is narrow-boiling behavior and the other is phase stability analysis.

Narrow-boiling behavior refers to the total enthalpy that is sensitive to temperature [32–37]. It is related to how the energy balance affects phase behavior in thermal compositional simulation. The limiting narrow-boiling behavior occurs for fluid systems with one degree of freedom, for which the enthalpy exhibits a discontinuity in temperature space [32,33,38–40].

Various researchers reported convergence difficulties associated

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* Corresponding author. Department of Petroleum and Geosystems Engineering, University of Texas at Austin, 200 E. Dean Keeton Street, Stop C0300, Austin, Texas 78712, USA.

E-mail address: okuno@utexas.edu (R. Okuno).

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with narrow-boiling behavior in their steam injection simulations [21,24,38,41]. The difficulties may be better handled in flow simulation with isobaric isenthalpic (PH) flash than with isobaric isothermal (PT) flash, because in the former type of thermal simulation formulation [e.g., 21, 38], narrow-boiling behavior is handled in local flash calculations that are decoupled from the global mass and energy flow equations. Even in stand-alone flash calculations, however, robust PH flash for narrow-boiling fluids has been a technical challenge [21,24,32–38]. It is not well understood under what thermodynamic conditions narrow-boiling behavior occurs; this question is addressed as one of the two main objectives in this research.

Recently, Zhu and Okuno [36,37] presented a robust direct substitution (DS) algorithm for PH flash for narrow-boiling fluids, including those with one degree of freedom. However, they did not study phase stability analysis in their PH flash. The assumption that the number of equilibrium phases is known is the major issue to be resolved for implementation of PH flash in flow simulation.

With the PH specification, the number of equilibrium phases is unknown not only in composition space, but also in temperature space. It can be determined at the solution temperature upon convergence. As presented in Brantferger [21,38], phase stability with PH specification can be analyzed only at a given temperature, which is not the equilibrium temperature until convergence.

Although phase stability analysis was not clearly described in most of the prior publications on thermal compositional simulation [e.g., 24, 29, 30, 31], it may be performed alternately with flash calculation for a fixed number of phases [21,38]. As in conventional PT flash, however, this sequential use of phase-stability and flash calculations is a series of local solutions, which requires obtaining false solutions and correcting them until the correct solution is obtained. Such PH flash becomes more difficult as the number of equilibrium phases increases because it tends to be attracted to a larger number of false solutions. It also becomes more difficult for a narrow-boiling fluid because false solutions at false temperatures may deviate substantially from the correct solution at the solution temperature for such a case.

Gupta et al. [33] proposed a novel formulation for PH flash that combines phase-stability and flash calculations. In their algorithm, the enthalpy, Rachford-Rice (RR), and stability equations were solved simultaneously for temperature, phase amounts, and stability variables. The stability variables of Gupta et al. [33] were derived from the first-order condition for unconstrained minimization of the Gibbs free energy as formulated by them. K values were updated in the outer loop based on the temperature change that was obtained from the internal iteration loop. It was reported that their algorithm could handle fluids with one degree of freedom. This is conceivable because the number of equilibrium phases is part of the solution in their PH flash [33]. To the best of our knowledge, the formulation and algorithm of Gupta et al.'s for PH flash have not been used in the literature since their original publication [33]. Various issues of their PH flash will be resolved in this paper, but briefly introduced here.

Firstly, non-convergence can occur when it attempts to solve the degenerate system of equations for a narrow-boiling fluid without using the method of Zhu and Okuno [36,37]. When narrow-boiling behavior occurs, it occurs within a phase region in which the number of phases is fixed. This is true even for the limiting case of one degree of freedom, for which the entire phase region of one freedom is narrow-boiling [e.g., a three-phase region (or point) for a binary system at a given pressure]. Thus, the coupling of phase-stability and flash calculations in itself does not necessarily improve the degeneracy issue associated with narrow-boiling behavior. Zhu and Okuno [36] presented non-convergence cases with the conventional PH flash algorithms even if the correct number of phases was used.

Secondly, it does not even start the iteration when the initial K values proposed by them yield ill-posed RR problems that have no solution. Their initial K values often form an unbounded feasible region for the RR solution. No solution exists for such a case, as proved by Okuno et al. [9].

Thirdly, their algorithm is initialized with an assumed maximum number of phases. During the iteration, if some of the phases (or iterative compositions) become close to one another, they are added together to decrease the number of iterative compositions. Subsequent computations are performed only for the distinct iterative compositions. That is, the number of iterative compositions only decreases, but does not increase, in their PH-flash algorithm. No scheme was proposed to handle the situation in which new phases appear in subsequent iterations as temperature changes in PH flash. This is problematic when the number and identities of phases change within the temperature domain of interest, as in steam injection simulation.

Fourthly, how to select a reference composition that was required to set the system of equations is unclear [33,42]. Alsaifi and Englezos [42] only stated in their paper on PT flash that a negative phase amount occurred when a reference composition was improperly selected.

Due to the various issues ranging from fundamental to implementation problems, no algorithm has been established for multiphase PH flash integrated with phase-stability analysis. In this paper, the coupling of phase-stability and flash calculations is reformulated on the basis of Brantferger's research on phase stability with PH specification [21,38]. Then, a new algorithm is presented to robustly solve the formulated multiphase PH flash. Also, a detailed analysis is given to address the unanswered question regarding thermodynamic conditions for narrow-boiling behavior. Case studies demonstrate that the developed algorithm can robustly perform multiphase PH flash integrated with phase-stability analysis even for narrow-boiling fluids, which none of the prior PH-flash algorithms [21,24,32–38] addressed in detail.

2. Formulation and algorithm

The new PH flash integrated with stability analysis is formulated by combining the conventional PH-flash formulation with the PT stability criterion that the tangent plane to the Gibbs free energy surface at a stable equilibrium state cannot lie above the Gibbs free energy surface at any composition. Then, a robust algorithm is developed for the formulated PH flash.

2.1. Formulation

The new formulation is a simple integration of the PH-flash formulation with Brantferger's analysis [21,38]. The correct phase equilibrium for a given P, $\underline{H}_{spec}$, and z_i ($i = 1, 2, \ldots, N_C$) is defined by a set of T and x_{ij} ($i = 1, 2, \ldots, N_C$, and $j = 1, 2, \ldots, N_P$) that gives the global maximum of the total entropy

$$\underline{S}^t = \sum_{j=1}^{N_P} \beta_j \underline{S}_j, \tag{1}$$

where P is pressure, $\underline{H}_{spec}$ is the specified molar enthalpy, z_i is the overall mole fraction of component i, T is temperature, x_{ij} is the mole fraction of component i in phase j, $\underline{S}^t$ is the total molar entropy, β_j is the mole fraction of phase j, $\underline{S}_j$ is the molar entropy of phase j, N_C is the number of components, and N_P is the number of equilibrium phases. The following constraints are to be satisfied: