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Robustness of three-phase equilibrium calculations

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ABSTRACT

Phase equilibrium calculations converge less often as the number of phases and components increase, and for overall compositions closer to phase split boundaries and critical points. Computational speed and robustness of flash calculations are very important aspects for pipeline transmission and for reservoir simulation where billions of flash calculations may be done. Reduced methods have the potential to improve the robustness of phase equilibrium calculations because if chosen properly they can linearize the equations, use fewer independent variables and can be unbounded. Improved robustness could further improve the speed and accuracy of compositional simulation and avoid false two-phase solutions, where three or more phases may be present.

In this paper, we use the reduced variables of Gorucu and Johns (2014) to test robustness in performing two- and three-phase stability analysis and corresponding flash calculations. These multi-phase equilibrium calculations are compared with the conventional phase equilibrium calculations based on minimization of Gibbs energy and the reduced method proposed by Okuno et al. (2010a). Using thousands of equally-spaced and unbiased multi-phase equilibrium calculations, the proposed multi-phase equilibrium calculations are shown to be more robust than the other two tested algorithms.

1. Introduction

Petroleum processes such as gas flooding or condensate gas/volatile oil production require compositional modeling where the movement of chemical components between the phases and in the reservoir must be tracked. A typical oil reservoir consists of thousands of hydrocarbon and nonhydrocarbon components that are lumped into few components and pseudocomponents. Although desirable for improved accuracy, simulation using many components is not practical with standard flash calculation procedures owing to large computational time. Current practice is to limit the number of defined and undefined components to between six and fifteen depending on how many heavy pseudocomponents (undefined components) are desired. Further, nearly all reservoir simulators do not perform three-phase flash calculations owing to their slow computational time, and increased likelihood of nonconvergence. The accuracy of reservoir simulations, however, decrease as more heavy components are lumped and/or as potential equilibrium phases are neglected.

There are likely an optimum number of components to use in simulation depending on computational speed, and the needed accuracy of the fluid modeled. Surface facility design for example generally requires a detailed fluid description of between 20 and 30 components. It would be desirable then to use 20 or more components to match those requirements, and to reduce errors in reservoir simulation associated with pseudocomponent lumping and neglected additional equilibrium phases. Reduced variables in phase behavior calculations are one possible approach to model more components and multiple phases in equilibrium more efficiently and robustly.

Phase equilibrium calculations become slower not only due to an increased number of components but also to an increased number of phases. The occurrence of a third hydrocarbon phase is common during low temperature gas injection, e.g. CO_2 injection in West Texas at temperatures less than about 100 °F where a CO_2-rich liquid phase, hydrocarbon-rich liquid phase and a vapor phase may appear (Turek et al., 1988), and also for injection of viscosity-reducing solvent in heavy oil reservoirs (Li et al., 2013). Calculations with an aqueous phase can also be important, adding the potential of four phases in equilibrium in some Permian basin CO_2 floods (Mohebbinia et al., 2013). Three-phase equilibrium calculations may also be important for CO_2 sequestration in oil reservoirs where the amount of CO_2 in the brine is of interest. Asphaltenes can also form during injection of volatile components

Abbreviations: BIP, Binary interaction parameters; ILJ, Our new algorithm based on Gorucu and Johns (2014); MG, Conventional method based on minimization of Gibbs energy; NR, Newton–Raphson; NEW, North Ward Estes; OJS, Algorithm based on Okuno, Johns and Sepehrnoori (2010a); SS, Successive substitution; TPD, Tangent plane distance

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Nomenclature

A	Attraction parameter
B	Repulsion parameter
e	ILJ residual function
J	Jacobian matrix
N_C	Number of components
N_p	Number of phases
Z	Compressibility factor
f	Fugacity
h_i	LJ vector
h	Independent variables for improved algorithms
G	Dimensionless molar Gibbs energy
g_i	LJ vector, gradient vector
K_i	K-value
k_{ij}	BIP matrix
n	Number of eigenvalues considered; iteration number
q	Eigenvector
$q_{i\alpha}$	Constant matrix of improved reduced methods
R	Residual function, convergence criterion
S	Stability analysis residual function
X	Stationary point
x	Liquid molar composition
y	Vapor composition
z	Overall composition

Greek letters

δ_1, δ_2	EOS parameters
ϕ	Fugacity coefficient
Θ	LJ reduced variables
λ	Eigenvalue
α	Reduced variable index
β	Phase mole fraction
ψ_k	Set of ILJ variables
ε	Convergence/switch tolerance

Subscripts

i	Composition
j	Composition or phase
L	Liquid
V	Vapor

so that five phases may coexist (Mohebbinia et al., 2014).

Phase equilibrium calculations usually consist of two basic steps: stability analysis and flash calculations. Stability analysis is used to save computational time by determining the number of stable equilibrium phases. Flash calculations then compute equilibrium phase compositions and phase mole fractions if stability analysis shows that a phase split should occur. Typically, phase equilibrium calculations begin by assuming a single phase exists in a given grid block and time step. If that phase is found unstable by stability analysis then two-phase flash calculations are carried out. A further check of stability is made on one of the two equilibrium phases. If unstable, a three-phase flash calculation should be done, although current practice is not to do this calculation because of increased computational time requirements and robustness of the calculations. Avoiding these calculations can result in significant inaccuracies in predicted recoveries (Okuno et al., 2010b). It would be advantageous therefore to have a robust and fast approach to three-phase (or more) equilibrium calculations.

Reduced methods can avoid excessive computational times when multiple phases and components are present. Previous research has proposed and analyzed reduced methods of various types (Michelsen, 1986; Hendriks, 1988; Hendriks and van Bergen, 1992; Jensen and Fredenslund, 1987; Li and Johns, 2006; Nichita et al., 2006; Okuno et al., 2010a; Nichita and Graciaa, 2010; Petitfrere and Nichita, 2015a). All of these aforementioned authors have focused on the computational speed or number of iterations of the reduced methods, and generally on only two-phase reduced methods. The robustness of two-phase flash calculations and stability analysis is critical to subsequent three-phase or even to four-phase flash calculations as the converged two-phase calculations are the initial input for subsequent multi-phase flash calculations.

While many reduced methods have been proposed and their computational speed improvements have been investigated, there has been very little research on the potential improved robustness of the reduced methods (Pan and Firoozabadi, 2002; Okuno, 2009; Gorucu and Johns, 2014, 2015). Pan and Firoozabadi (2002) analyzed the tangent plane distance (TPD) for an example fluid and concluded that the reduced method had only one minimum in reduced space, while the conventional technique in compositional space had two observable minima for the fluid tested. This conclusion has been questioned by Haugen and Beckner (2013) who stated that the reduced number of minima may be related to a small change in phase behavior owing to the reduced technique used (eigenvalue decomposition where small eigenvalues are set to zero). Okuno et al. (2009, 2010a), however, reported the number of failed flash calculations as the number of components increases and showed that the number of convergence failures were significantly larger with conventional techniques. In their reduced approach the phase behavior predictions were identical between the conventional and reduced methods so that the improvement in robustness was more certain, at least for the fluids studied. Recently, Petitfrere and Nichita (2015b) introduced a new multiphase equilibrium calculation technique using a reduction method which is very similar to our algorithm (Gorucu, 2013). In their paper, they also show that their reduction method is equivalent to an unbounded minimization problem. However, Petitfrere and Nichita implemented reduced parameters based on eigenvalue decomposition, which has been shown to be significantly slower than when the empirical BIP formula of Li and Johns (2006) is used (Gorucu and Johns, 2015).

Because the reduced methods decrease the number of independent variables, the reduced methods could exhibit less complicated behavior compared to the conventional technique owing to significantly smaller search space (five-component space with Li and Johns (2006) reduced variables compared to NC hyperspace with conventional methods). Gorucu and Johns (2015) implemented published two-phase reduced and conventional flash calculations and compared these techniques in terms of speed and robustness. Their results for the numerous fluids studied showed that the reduced variables of Nichita and Graciaa (2011) were more robust compared to other reduced and conventional techniques likely because of the linearization of the fugacity expression. Gorucu and Johns results were based on thousands of unbiased two-phase flash calculations.

In this paper, we focus on the improvement in robustness of published three-phase reduced methods. First, we briefly describe our algorithm for conventional phase equilibrium calculations. Then, we implement the reduced variables of Gorucu and Johns (2014) for both stability analysis and three-phase flash calculations. We then give our methodology to test and compare the