

# Application of a Reduced Method in Compositional Simulation

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## Summary

Simulating gas-injection processes requires a compositional model to predict the fluid properties resulting from mass transfer between reservoir fluid and injection gas. A drawback of compositional simulation is the efficiency and robustness of phase equilibrium calculations. Reduced methods for phase equilibrium calculations have been studied as a potential solution to improve the efficiency of compositional simulation. However, most of those studies have been performed only in standalone calculations, and the robustness and efficiency of a reduced method has not been confirmed in compositional simulation. In this research, we develop a robust and efficient algorithm for a reduced method and validate it in compositional simulation.

We examine the efficiency and convergence property of the conventional algorithm for a reduced method and solve several implementation problems in a compositional simulator. The reduced method is implemented in UTCOMP, a compositional implicit-pressure/explicit concentration (IMPEC) simulator, to demonstrate the performance for various numbers of components and degrees of miscibility. The results show that the reduced method enables significant savings in execution time of compositional simulation without loss of accuracy compared to standard methods. Also, we observe that the reduced method exhibits improved robustness, especially for miscible processes where composition paths go near critical regions.

## Introduction

Phase-behavior algorithms can significantly affect the efficiency and reliability of compositional simulation. This is because most phase-behavior algorithms iteratively solve nonlinear equations to predict the number of coexisting phases and phase properties. Phase-behavior calculations become more difficult, time-consuming, and important as multicontact miscibility is approached.

Phase-behavior calculations in compositional simulation consist of stability analysis and flash calculations. To improve the efficiency of the flash calculations, a noniterative procedure was developed by Stenby and Wang (1993). They concluded that their procedure can decrease the simulation time usually by a factor of two with reasonable accuracy. However, because their noniterative procedure approximates phase compositions and amounts on the basis of linear extrapolation from the previous timestep, the simulation accuracy is highly problem-dependent. For example, the procedure could cause significant errors in simulation of miscible-gas injection with a large number of grid cells, large timesteps, and a long simulation period. Such a difficult case for the noniterative procedure was not tested in their paper.

A desirable approach to an efficient simulation is to reduce computational time without loss of accuracy. A reduced method that originated with Michelsen (1986) has been studied as a potential solution. One of the main problems with the development of reduced methods was how to handle nonzero binary interaction coefficients (BICs) (Jensen and Fredenslund 1987; Hendriks 1988; Hendriks and van Bergen 1992; Kaul and Thrasher 1996). Li and Johns (2006) proposed an approach in which two sets of component-specific parameters were introduced to develop the BIC matrix. In this

research, we use Li and Johns' approach because of its simplicity and flexibility.

Other previous studies on reduced methods include comparisons of algorithms, as well as application to stability analysis and multiphase calculations (Firoozabadi and Pan 2002; Nichita et al. 2002, 2006; Pan and Firoozabadi 2003; Hoteit and Firoozabadi 2006). A few papers reported implementation of a reduced method in a compositional simulator, but only for flash calculations, not stability analysis. Wang and Barker (1995) applied Michelsen's reduced flash (RF) calculations in a compositional simulator, concluding that the RF does not offer significant savings in simulation time. Honami et al. (2000) reported simulation case studies using RF calculations in which simulation results were different from those with a commercial simulator.

To the best of our knowledge, no paper reports the efficiency and robustness of reduced methods applied to both stability and flash calculations in compositional simulation. In this research, we improve problems of currently used algorithms for reduced stability and flash calculations. Then, we implement the improved reduced method in a compositional simulator to demonstrate conclusively the efficiency and robustness of our method.

## Formulation and Algorithms

In this section, we present the reduced parameters used in this research. We then derive formulations of the reduced flash and stability analysis and present practical algorithms to solve the formulated problems.

**Reduced Parameters.** The Peng-Robinson equation of state (EOS) (Peng and Robinson 1976) is used with the van der Waals mixing rules throughout this research, although any cubic EOS can be used. To handle nonzero BICs, Li and Johns (2006) introduced two sets of component-specific parameters to replace BICs:

$$k_{ij} = (h_i - h_j)^2 g_i g_j$$

and

$$i, j = 1, \dots, N_c.$$

The parameters  $h_i$  and  $g_i$  can be considered as fitting parameters to represent the BICs or, better yet, to match pressure/volume/temperature (PVT) data directly; the parameters  $h_i$  and  $g_i$  could replace BICs during fluid characterization. As long as the characterized fluid model using the parameters  $h_i$  and  $g_i$  can predict the phase behavior accurately, the reduced phase-equilibrium calculations are as accurate as the conventional calculations. The reduced parameters are defined as  $\theta_k^L = \sum_{i=1}^{N_c} \eta_{ki} x_i$  for a liquid phase and  $\theta_k^V = \sum_{i=1}^{N_c} \eta_{ki} y_i$  for a vapor phase, where  $\eta_i = (B_i, \sqrt{A_i}, \sqrt{A_i} h_i g_i, \sqrt{A_i} h_i^2 g_i, \sqrt{A_i} g_i)$ , and  $k = 1, \dots, 5$ .

Fugacity coefficients for a phase can be expressed as functions of the five reduced parameters for the corresponding phase (see Appendix A). As described later, the numbers of independent variables for the reduced flash and stability analysis are six and five, respectively, regardless of the number of components ( $N_c$ ). Therefore, the reduced method can decrease the dimension of the system of equations to be solved when more than six components are used in the calculations. The reduced dimension can be exploited when the Newton method is used to solve either the stability analysis

or flash calculations. In this research, the reduced method is applied with the Newton method and initiated by the conventional successive substitution (SS) both for stability analysis and flash calculations. This successive use of SS and the Newton method is commonly applied in compositional reservoir simulation because the Newton method is quadratically convergent only when a good initial estimate of the parameters is given. SS is linearly convergent with a much larger region of convergence compared to the Newton method.

**Reduced Flash Calculations.** We now derive a practical and robust algorithm for two-phase reduced flash calculations. The most fundamental formulation for flash calculations at given temperature and pressure is minimization of the Gibbs free energy. An alternative and conventional formulation is to solve a system of fugacity equations, which corresponds to the first-order necessary condition of the minimization of the Gibbs free energy. In this research, our formulation is based on the fugacity equations. The flash calculation is to solve the following equations:

Fugacity equations:

$$F_i = \ln f_i^L - \ln f_i^V = 0 \quad (i = 1, \dots, N_c) \quad \dots \dots \dots (1)$$

Component material balance equations:

$$z_i = Lx_i + Vy_i \quad (i = 1, \dots, N_c) \quad \dots \dots \dots (2)$$

Overall material balance equation:

$$L + V = 1 \quad \dots \dots \dots (3)$$

Summation conditions:

$$\sum_{i=1}^{N_c} x_i = \sum_{i=1}^{N_c} y_i = 1. \quad \dots \dots \dots (4)$$

In a conventional flash algorithm, the above equations are solved with  $N_c$  independent variables (Fussell and Yanosik 1978; Nghiem et al. 1983).

Rearranging Eq. 1,  $K$  values become functions of 10 reduced parameters.

$$K_i \equiv y_i/x_i = \varphi_i^L(\theta^L)/\varphi_i^V(\theta^V) \quad (i = 1, \dots, N_c). \quad \dots \dots \dots (5)$$

Considering the material balance Eqs. 2 and 3,  $\theta_k^V$  can be expressed using  $\theta_k^L$  and  $L$ .

$$\theta_k^V = (\theta_k^z - L\theta_k^L)/(1-L), \quad \dots \dots \dots (6)$$

where  $\theta_k^z = \sum_{i=1}^{N_c} \eta_{ki} z_i$  and  $k = 1, \dots, 5$ . Therefore,  $K$  values are functions of the six parameters,  $L$  and  $\theta_k^L$  ( $k = 1, \dots, 5$ ). Once  $K$  values are calculated, phase compositions are computed directly as

$$x_i = z_i/[L + K_i(1-L)] \text{ and } y_i = K_i x_i, \quad \dots \dots \dots (7)$$

where  $i = 1, \dots, N_c$ . Because phase mole fractions and component mole fractions are functions of the six parameters, the flash calculations can be formulated in terms of the six independent variables. Component mole fractions calculated by Eq. 7 do not necessarily satisfy Eq. 4. In the reduced method, Eq. 4 is satisfied once convergence is achieved because it is part of the system of equations to be solved as described later.

The nonlinear equations to be solved in the reduced flash are

$$F_k^R(\underline{\psi}) = \psi_k - \sum_{i=1}^{N_c} \eta_{ki} x_i = 0$$

and

$$F_6^R(\underline{\psi}) = \sum_{i=1}^{N_c} (x_i - y_i), \quad \dots \dots \dots (8)$$

where  $\underline{\psi} = (\theta_1^L, \theta_2^L, \theta_3^L, \theta_4^L, \theta_5^L, L)$  and  $k = 1, \dots, 5$ . The Jacobian matrix is 6x6 regardless of  $N_c$  used in the flash calculations. Therefore,

solution of a system of equations by the Newton method is faster for the RF than that for the conventional flash for fluids with more than six components.

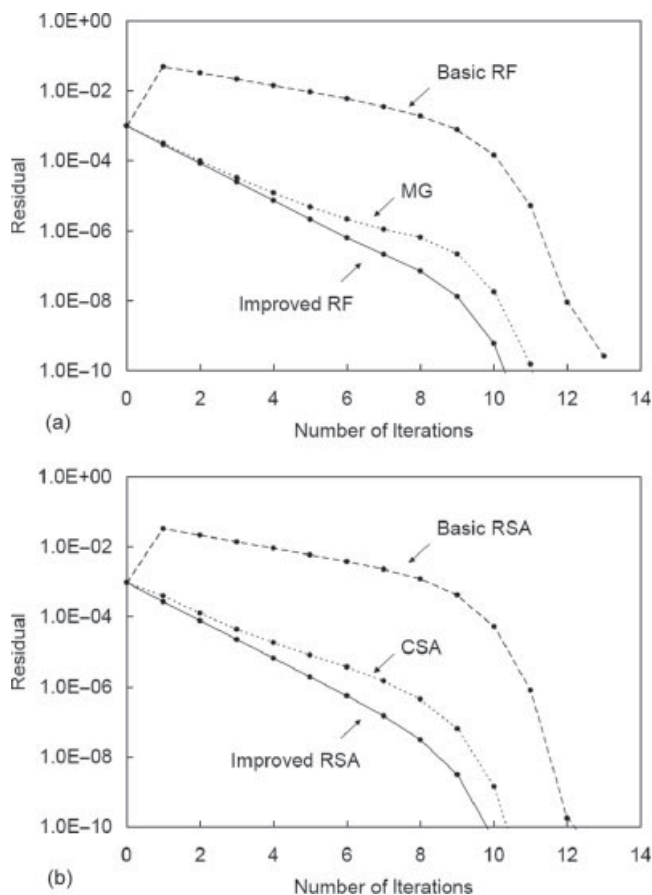
The algorithm developed for the RF is as follows:

1. Calculate  $\theta_k^z$  ( $k=1, \dots, 5$ ).
2. Obtain initial estimates for the six independent variables,  $\psi_j$  ( $j=1, \dots, 6$ ), based on the solution from successive substitution.
3. Calculate  $\theta_k^V$  ( $k=1, \dots, 5$ ) using Eq. 6.
4. Calculate compressibility factors and fugacity coefficients for liquid and vapor phases using the EOS. When the cubic EOS has multiple roots of the compressibility factor, the correct root is selected that results in the lowest Gibbs free energy (Evelein et al. 1976).
5. If  $\max\{|F_i|\} < \varepsilon$ , stop; otherwise, continue to Step 6.
6. Calculate  $K$  values using Eq. 5 based on the fugacity coefficients in Step 4.
7. Calculate compositions for liquid and vapor phases using Eq. 7.
8. Calculate the residuals of Eq. 8.
9. Construct the 6x6 Jacobian matrix analytically (see Li and Johns 2006) and solve the system of equations.
10. Update the six independent variables  $\psi_j$  ( $j=1, \dots, 6$ ).
11. Repeat Steps 3, 4, 6, and 7, and update the independent variables except for  $\psi_6 (=L)$ .
12. Go to Step 3.

The above algorithm is different from that of Li and Johns (2006), which uses the basic Newton method to solve the system in the reduced space (i.e., go to Step 3 after Step 10). As will be shown, the above algorithm improves the convergence behavior near critical points. Also, the stopping criterion is based on the fugacity equations alone in the above algorithm. This is an important issue in practice and will be discussed in the Simulation Case Studies section.

To demonstrate the improved convergence behavior of our algorithm for RF calculations (improved RF), we compare it with the following three algorithms: the basic algorithm for RF calculations (basic RF) (Li and Johns 2006), minimization of the Gibbs free energy with respect to component mole numbers in a phase (MG) (Perschke et al. 1989), and solution of fugacity equations with respect to  $K$  values (FK) (Nghiem et al. 1983). **Fig. 1** shows the convergence behaviors in terms of the residuals of the fugacity equations, Eq. 1, with different algorithms. The fluid used is Oil A of Li and Johns (2006) at 484°F and 1,044.62 psia for a near-critical mixture (**Table 1**). The initial estimates are given by SS with a switching criterion to the Newton iteration when  $\max\{|F_i|\} < 10^{-3}$ . The convergence rate for each algorithm is linear for the first eight iterations, indicating that the switching point from SS to the Newton method is not within the region of the quadratic convergence of the Newton method. Nevertheless, the Newton method should be used in the final iterations because using SS alone requires more than 78,000 iterations to reduce  $\max\{|F_i|\}$  from  $10^{-3}$  to  $10^{-8}$ , compared to 10 iterations for the improved RF. The basic RF can take almost twice the number of iterations compared with the improved RF when a stopping criterion of  $\max\{|F_i|\} < 10^{-6}$  is used. The behavior of the basic RF results from the fact that the reduced method solves the fugacity equations, Eq. 1, only indirectly. The improved RF also solves the fugacity equations indirectly, but the improved algorithm eliminates the undesirable convergence behavior. The convergence behavior of our improved RF is remarkable considering its simplicity because it can converge with a smaller number of iterations than MG, which uses a line-search technique to enhance the convergence. FK is not shown in the figure because, for this case, it converges to the trivial solution where the vapor- and liquid-phase compositions are identical. Although the improved RF requires 20% more calculation time per iteration than the basic RF, the tradeoff is worth the increased robustness.

When implemented in a simulator, we found that the improved RF rarely converged to the trivial solution for extremely difficult cases in which overall compositions are very near the binodal curve in the critical region. For these few cases, the flash calculation is repeated where the Rachford-Rice equation (1952) is solved in Step 11 to obtain phase compositions and mole fractions and update the six independent variables. This procedure makes the



**Fig. 1—Comparisons of the convergence behaviors of different algorithms for a near-critical mixture. (a) Flash calculations. (b) Stability analysis.**

summation conditions, Eq. 4, satisfied at each iteration and tends to avoid the trivial solution. Besides, one may avoid the trivial solution by selecting the independent variables between  $(\theta_1^L, \dots, \theta_5^L, L)$  and  $(\theta_1^V, \dots, \theta_5^V, V)$  on the basis of values of  $L$  and  $V$  (Fussell and Yanosik 1978).

**Reduced Stability Analysis.** In this section, we derive an algorithm for stability analysis using the reduced method. A common numerical method for stability analysis is to search for a phase composition at which the tangent plane distance (TPD) function is negative (Michelsen 1982). If such a phase composition is found, the current phase with composition  $\underline{z}$  is unstable. Otherwise, the current phase is assumed to be stable. The stationary point method of Michelsen locates stationary points on the TPD function and checks the sign of the TPD function to identify phase stability.

For stability analysis of a single-phase mixture, the location of stationary points is performed using vapor- and liquid-like

initial estimates based on  $K$  values from Wilson's correlation (1969). If the first calculation with a vapor-like (or liquid-like) estimate converges either to the trivial solution or to a nontrivial solution with a positive value of the TPD function, then the second calculation starts with a liquid-like (or vapor-like) estimate searching for phase instability. If the two calculations do not identify phase instability, the current phase with composition  $\underline{z}$  is assumed to be stable. If either set of the calculation identifies phase instability, the stability analysis is followed by a flash calculation to obtain the two-phase solution. An integral part of the algorithm is to locate stationary points, and the reduced method can be applied there. The following stationarity equations should be satisfied at a stationary point of the TPD function:

$$S_i = \ln X_i + \ln \varphi_i(\underline{x}) - \ln z_i \varphi_i(\underline{z}) = 0 \quad (i = 1, \dots, N_c) \quad (9)$$

In a conventional algorithm, Eq. 9 is solved with the independent variables of  $X_i$  ( $i=1, \dots, N_c$ ). The mole fractions are calculated as

$$x_i = X_i / \sum_{j=1}^{N_c} X_j \quad (i = 1, \dots, N_c) \quad (10)$$

Rearranging Eq. 9, all variables are functions of the five reduced parameters. That is,

$$X_i = z_i \varphi_i(\underline{z}) / \varphi_i(\underline{\theta}) \quad (11)$$

and we need only five equations to solve the original problem of  $N_c$  dimensions. The nonlinear equations to be solved for reduced stability analysis are

$$S_k^R(\underline{\theta}) = \sum_{i=1}^{N_c} (\theta_k - \eta_{ki}) z_i \varphi_i(\underline{z}) / \varphi_i(\underline{\theta}) \quad (k = 1, \dots, 5) \quad (12)$$

The size of the Jacobian matrix is  $5 \times 5$  regardless of  $N_c$ , which makes the solution of a system of equations faster for the reduced method than for the conventional method. The reduced method is switched from SS when a specified criterion is satisfied (e.g.,  $\max\{|S_i^R|\} < 10^{-3}$ ). The algorithm for locating a stationary point using the reduced method is as follows:

1. Calculate compressibility factors and fugacity coefficients for the phase with composition  $\underline{z}$ . When the cubic EOS has multiple roots in the compressibility factor, the correct root is selected to result in the lowest Gibbs free energy (Evelein et al. 1976). This is also true for Step 5 below.
2. Obtain initial estimates for  $X_i$  ( $i=1, \dots, N_c$ ) from successive substitution.
3. Calculate mole fractions using Eq. 10.
4. Calculate the five reduced parameters.
5. Calculate compressibility factors and fugacity coefficients for the phase with composition  $\underline{x}$  as functions of  $\underline{\theta}$ .
6. If  $\max\{|S_i^R|\} < \epsilon$ , stop; otherwise, continue to Step 7.
7. Calculate residuals of Eq. 12.
8. Construct the  $5 \times 5$  Jacobian matrix analytically (see Okuno 2009) and solve the system of equations.
9. Update the five reduced parameters.

**TABLE 1—EOS PARAMETERS FOR OIL A\***

	Mole fraction (Mol %)	$T_c$ (°F)	$P_c$ (psia)	Acentric factor	$h$	$g$	BIC CO <sub>2</sub> **	BIC C <sub>1</sub> **	BIC n-C <sub>10</sub> **
CO <sub>2</sub>	5.0	87.90	1069.87	0.225	1.0	1.170	0.000	0.144	0.114
C <sub>1</sub>	10.0	-116.59	667.20	0.008	0.3	0.250	0.144	0.000	0.071
C <sub>2</sub>	12.0	90.05	708.35	0.098	0.0	0.103	0.120	0.002	0.040
C <sub>3</sub>	12.0	205.97	615.76	0.152	0.0	0.103	0.120	0.002	0.040
n-C <sub>4</sub>	15.0	305.69	551.10	0.193	0.0	0.103	0.120	0.002	0.040
n-C <sub>5</sub>	17.0	385.61	489.38	0.251	0.0	0.103	0.120	0.002	0.040
n-C <sub>10</sub>	29.0	652.01	305.68	0.490	2.0	0.098	0.114	0.071	0.000

\* From Li and Johns (2006).

\*\* All others are 0.0.



10. Repeat Step 5 and calculate  $X_i (i=1, \dots, N_c)$  using Eq. 11.

11. Go to Step 3.

The algorithm presented here is different from the basic Newton method to solve the system in the reduced space (i.e., go to Step 5 after Step 9). A main difference is that our algorithm takes one SS step inside the iteration loop, which improves the convergence behavior near critical points.

Fig. 1 compares the convergence behaviors in terms of residuals of the stationarity equations, Eq. 9, with the following algorithms: the improved algorithm for reduced stability analysis (improved RSA), the basic Newton method to solve the reduced system Eq. 12 (basic RSA), and the conventional stability analysis with direct solution of the stationarity equations with respect to the  $N_c$  independent variables (CSA). The fluid used in the comparison is Oil A of Li and Johns (2006) for a near-critical mixture (Table 1). The initial

estimate for the Newton iteration of the stability analysis is given by SS with a switching criterion of  $\max\{|S_i|\} < 10^{-3}$ . Both the basic and improved RSA solve the stationarity equations only indirectly, but the improved RSA does not exhibit the undesirable convergence behavior of the basic RSA as shown in Fig. 1. Although the improved RSA requires 30% more calculation time per iteration than the basic RSA, the tradeoff is worth the increased robustness. The results show that the basic RSA can take almost twice the number of iterations compared with the improved RSA when a stopping criterion of  $\max\{|S_i|\} < 10^{-6}$  is used. The improved RSA can converge in an even smaller number of iterations than CSA, which directly solves the stationarity equations with the  $N_c$  independent variables.

Hoteit and Firoozabadi (2006) reported that the minimum of the TPD function obtained by local minimization algorithms can be discontinuous in a single-phase region in P-T space. They also reported that numerical algorithms for stationary points can exhibit poor convergence behavior near the discontinuity. However, they did not discuss what causes the discontinuity and convergence problems. In Appendix B, we demonstrate the appearance of the discontinuity for a binary mixture as the pressure changes at a fixed temperature. The poor convergence can result from a saddle point on the TPD function. A saddle point appears at the outer boundary of the “shadow-phase region” of Rasmussen et al. (2006). The shadow-phase region is where Eq. 9 has two solutions—the trivial solution and a nontrivial solution with a positive value for the TPD function. Although several potential remedies for the convergence problem are discussed in Appendix B, we implement the procedure of Hoteit and Firoozabadi (2006). The maximum number of iterations is limited to 15, and the single-phase mixture of interest is assumed to be stable when convergence cannot be achieved within the maximum number of iterations.

### Comparisons in Standalone Calculations

As described in the previous section, the reduced method solves equations that are not directly related to the fugacity equations, Eq. 1, for flash calculations, and stationarity equations, Eq. 9, for stability analysis. Although Fig. 1 demonstrated that the improved reduced method can converge in fewer iterations than other algorithms for the same initial estimate, we investigate further the robustness and efficiency of the reduced method. From this point on, we consider only the improved RF and the improved RSA.

**Robustness.** For flash calculations, we compare the robustness of the algorithms RF and FK, both of which use a simple solution of the nonlinear equations using the Newton method. The comparisons are based on the number of SS steps required for the Newton method to converge to a correct solution. A smaller number of SS steps required would indicate that the function behaves favorably for the Newton method within a wider region around the solution. Flash calculations for Oil A (Table 1) are performed at different conditions along the line on the P-T diagram shown in Fig. 2. The initial estimates used in the calculations are generated by Wilson’s correlation (1969). As shown in Fig. 2, the number of SS steps required is a strong function of the distance from the critical point. RF requires a smaller number of SS steps than FK at all the conditions studied here. The advantage of RF against FK becomes significant in the critical region. This behavior is favorable because robustness of algorithms in the critical region is important in the simulation of gas injection where the compositional path can go near or through the critical region.

For stability analysis, we compare RSA with CSA. The comparisons are based on the number of iterations taken by the Newton method. The initial estimates are again generated by Wilson’s correlation. Fig. 2 shows that the number of iterations increases as the conditions become close to the critical region. CSA converges in up to twice the number of iterations compared with RSA, indicating the robustness of the reduced method. It should be noted that both algorithms need no SS step for the Newton iteration to converge to a correct solution for all conditions studied here.

**Efficiency.** The total calculation time of an iterative standalone algorithm is approximately a product of the calculation time per

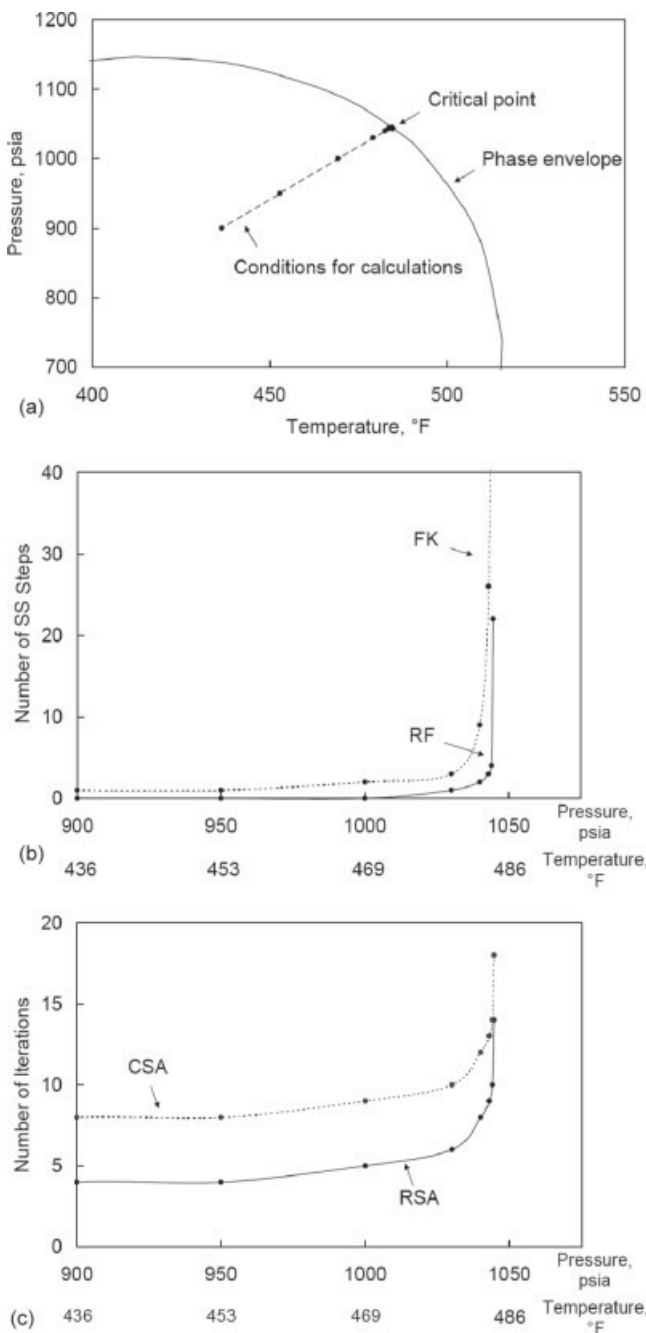


Fig. 2—(a) P-T diagram of Oil A showing the conditions used in the comparisons. (b) The number of SS steps required for the second-order flash algorithms to converge. (c) The number of iterations taken by different second-order algorithms for stability analysis.

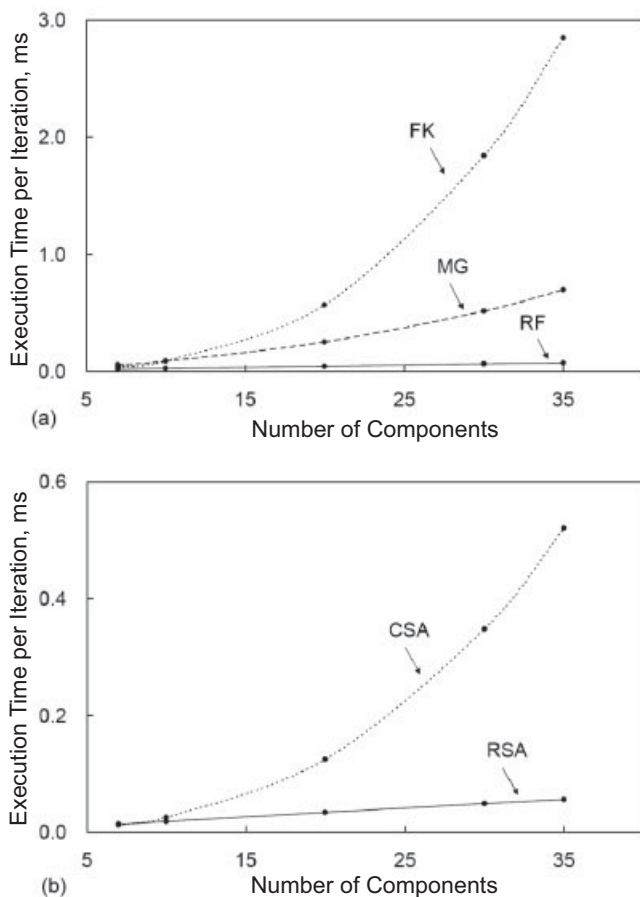


Fig. 3—Execution time per iteration with different algorithms. (a) Flash calculations. (b) Stability analysis.

iteration and the number of iterations. As shown in Figs. 1 and 2, the reduced method generally takes a smaller number of iterations than the others. Therefore, comparisons of calculation time per iteration would demonstrate the efficiency of the reduced method in standalone calculations. The computations are performed using a Pentium 4 processor at 3.0 GHz and 2.0 GB of RAM throughout this research.

A significant part of calculation time per iteration can be spent in construction of the Jacobian or Hessian matrix, and solution of the systems by the Newton method. The reduced method decreases the calculation time by decreasing the size of the Jacobian matrix. We again use Oil A. Fig. 3 shows that the calculation time per iteration is much shorter for the reduced method than for the others. The advantage of the reduced method increases rapidly with  $N_c$  because the number of equations to be solved is fixed for the reduced method, while those for MG and FK increase with  $N_c$ . The results are consistent with an algebraic fact that, if a direct solver is used, the solution of the system of equations requires operation counts on the order of the cube of the number of equations.

The significant speed-up of the reduced method is not only because of the rapid solution of the system of equations, but also because of rapid construction of the Jacobian matrix. Rasmussen et al. (2006) stated that construction of the Jacobian matrix for a reduced method is cumbersome. Fig. 4 compares the calculation time spent in the construction of the Jacobian or Hessian matrix for different algorithms for flash and stability analysis. The calculation time spent in the construction of such a matrix is shorter for the reduced method for all cases except for the seven-component stability analysis case. The computational cost of construction of the Jacobian or Hessian matrix depends on how directly the functions are related to the independent variables. The reduced parameters explicitly express fugacity coefficients, which are important thermodynamic state functions in phase equilibrium calculations

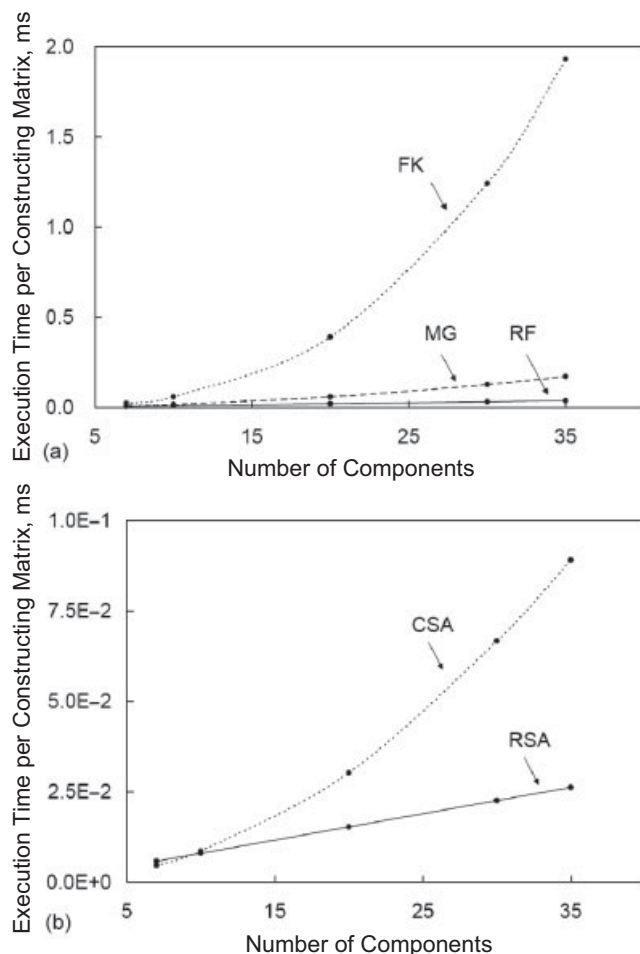


Fig. 4—Execution time for constructing matrices with different algorithms. (a) Flash calculations. (b) Stability analysis.

(see Appendix A). In Fig. 4, the Jacobian matrix construction in FK is more time-consuming than those in the other algorithms. This is because  $K$  values are related to fugacity in a significantly indirect manner. The construction of the Hessian matrix in MG is computationally inexpensive because the matrix is symmetric and because the function has a relatively direct relation to the independent variables.

### Simulation Case Studies

Standalone calculations are necessary but not sufficient for the algorithms to be practically workable in a simulator. The algorithms developed in this research are implemented in UTCOMP, which is an IMPEC compositional simulator originally developed by Chang et al. (1990). Perschke et al. (1989) developed the phase-behavior algorithms in the original UTCOMP. The algorithms consist of accelerated SS and minimization of the Gibbs free energy for flash calculations, and the stationary point method and minimization of the TPD function for stability analysis. All the calculations are performed in conventional  $N_c$  space. In this research, we replaced the accelerated SS with the normal SS to robustly initiate the second-order convergence method.

The main factors making phase-equilibrium calculations time-consuming and difficult are the number of components and the degree of miscibility. To demonstrate the robustness and efficiency of the reduced method, simulation case studies are conducted using UTCOMP with three different combinations of the algorithms: (RSA, RF), (CSA, MG), and (CSA, FK). Gas injection in a quarter five-spot pattern with a stochastically generated permeability field is simulated with a varying number of components and degree of miscibility using a 2D reservoir model. The reservoir properties and fluid properties are summarized in Tables 2 and 3, respectively.

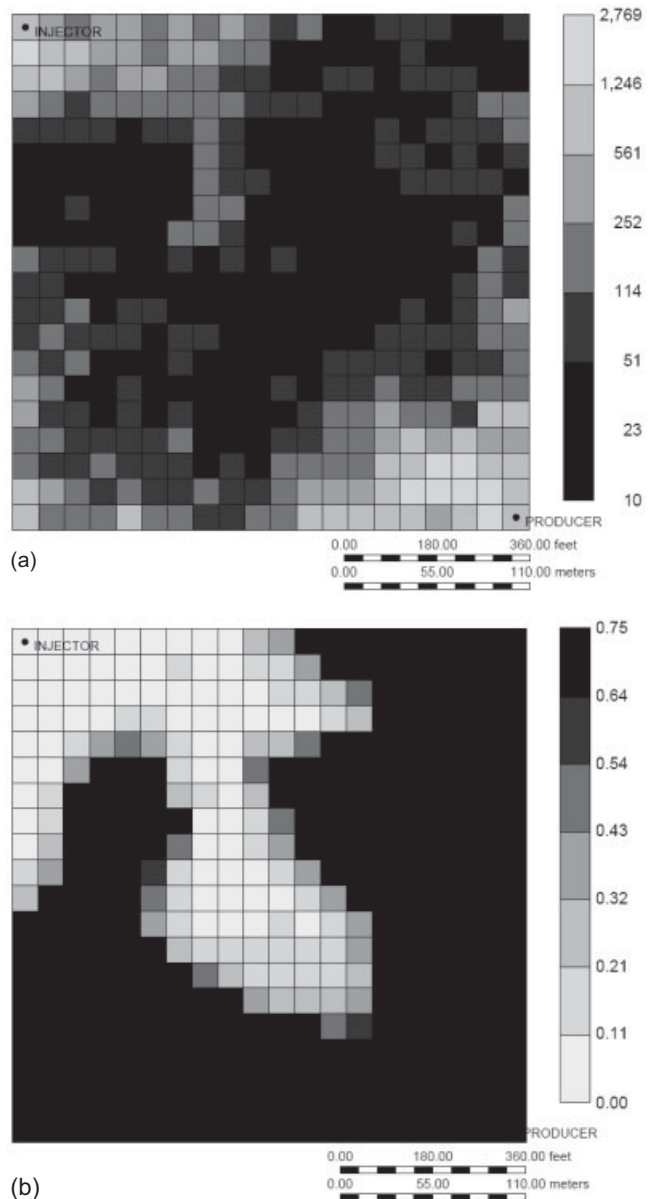
**TABLE 2—RESERVOIR PROPERTIES IN THE SIMULATION CASE STUDIES**

Dimensions	1,000×1,000×20 ft
Number of grid cells	20×20×1
Porosity	0.25
Mean permeability	113 md
Dykstra-Parsons coefficient	0.74
Correlation length	300 ft
Reservoir temperature (water/oil/gas)	260°F
Residual saturation (water/oil/gas)	0.25/0.20/0.05
Endpoint relative permeability (water/oil/gas)	0.21/0.70/0.35
Exponent of Corey model (water/oil/gas)	1.5/2.5/2.5
Initial saturation (water/oil/gas)	0.25/0.75/0.00

The permeability field used and an oil saturation distribution before breakthrough are shown in Fig. 5. The number of components is varied from 7 to 20. When more than seven components are used, the heaviest pseudocomponent,  $C_{25+}$ , is split to as many components as needed with the same properties. The degree of miscibility is varied by changing reservoir pressure at a constant temperature of 260°F. The minimum miscibility pressure (MMP) calculated by the PVTsim software of Calsep is 3,626 psia at the reservoir temperature. In each case, the injection gas is injected for one pore volume (PV).

For stability and flash calculations, the second-order convergence methods are initiated by SS. The switching criteria are  $\max\{|S_i|} < 10^{-3}$  for stability analysis and  $\max\{|F_i|} < 10^{-3}$  for flash calculations. The stopping criteria of the Newton methods are  $\max\{|S_i|} < 10^{-8}$  for stability analysis and  $\max\{|F_i|} < 10^{-8}$  for flash calculations. In addition, CSA, MG, and FK use a relative step size criterion,  $\max\{|\delta\alpha_i/\alpha_i|\} < 10^{-8}$ , where  $\alpha_i$  is the  $i$ th independent variable and  $\delta\alpha_i$  is the updated amount for  $\alpha_i$ . The stopping criteria for the reduced method are based neither on the residuals of the reduced equations, Eqs. 8 and 12, nor on the relative step size. That is, the RF uses residuals of fugacity equations alone as the stopping criterion. We observed a case in which the maximum norm of the reduced flash equations is  $10^{-9}$ , while that of fugacity equations is  $10^{-3}$ . Pan and Firoozabadi (2003) reported similar observations. Therefore, the residuals of the reduced equations should not be used for determination of convergence of the reduced method.

One of the popular algorithms for stability analysis is a quasi-Newton method to minimize the TPD function using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method for the inverse of the Hessian matrix approximation (Michelsen 1982). The BFGS quasi-Newton method is superlinearly convergent at best and can avoid solution of the system of equations at the expense of curvature information used in the iteration. That is, the BFGS quasi-Newton method can take more iterations than the Newton method at less computational effort per iteration. Ammar and Renon (1987) compared various algorithms for minimization of the Gibbs free



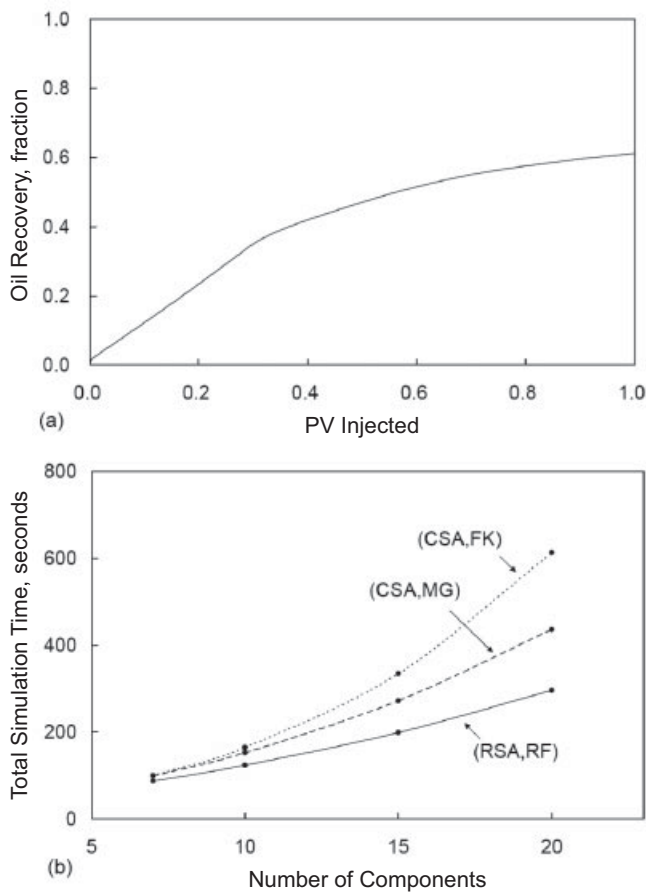
**Fig. 5—(a) Randomly generated permeability field in md. (b) Oil saturation distribution at 0.25 PV for the immiscible case.**

energy including the Newton and BFGS quasi-Newton methods. Their comparisons showed that the Newton method requires shorter execution time than the BFGS quasi-Newton method in all cases studied in their paper. In this research, we do not consider the BFGS quasi-Newton method both for stability analysis and flash calculations, although it can be applied to both conventional

**TABLE 3—FLUID PROPERTIES USED IN SIMULATION CASE STUDIES**

	Oil (Mol %)	Gas (Mol %)	Molecular weight	$T_c$ (°F)	$P_c$ (psia)	Acentric factor	$h$	$g$	BIC CO <sub>2</sub> *
CO <sub>2</sub>	0.77	1.0	44.01	87.90	1071.60	0.225	1	1	0
C <sub>1</sub>	20.25	65.0	16.04	-116.59	667.20	0.008	0	0.1318	0.1318
C <sub>2-3</sub>	11.80	30.0	38.40	158.88	653.37	0.130	0	0.1318	0.1318
C <sub>4-6</sub>	14.84	4.0	72.82	379.87	485.94	0.244	0	0.1318	0.1318
C <sub>7-14</sub>	28.63	0.0	135.82	625.86	351.54	0.600	0	0.09885	0.09885
C <sub>15-24</sub>	14.90	0.0	257.75	861.15	261.51	0.903	0	0.09885	0.09885
C <sub>25+</sub>	8.81	0.0	479.95	1202.09	250.31	1.229	0	0.09885	0.09885

\* All others are 0.0.



**Fig. 6—Comparisons for the immiscible case. (a) Oil recovery is identical for all algorithms. (b) Total simulation time vs.  $N_c$  for the different combinations of flash and stability algorithms.**

and reduced methods. We investigate the effect of the number of equations to be solved for phase-equilibrium calculations on the efficiency of reservoir simulation, instead of the effect of the convergence rate near the solution or the curvature information used in the iteration.

In the simulation case studies, stability analysis for a single phase is performed only for well cells and cells adjacent to two-phase cells. Flash calculations are performed for grid cells where two phases existed at the previous timestep or stability analysis indicates instability of a single phase.

**Immiscible Case.** For this case, the initial, injection, and production pressures are set to 2,850, 2,900, and 2,400 psia, respectively. This case is relatively easy for phase-equilibrium algorithms because the thermodynamic conditions are far from miscibility. All algorithms converge with no failures and lead to exactly the same simulation results (**Fig. 6**). Location of a stationary point for stability analysis was performed approximately 100,000 times,

and flash calculations were performed approximately 400,000 times. Average numbers of iterations for RSA, CSA, RF, MG, and FK were 1.9, 2.0, 1.6, 1.6, and 1.8, respectively. **Table 4** shows a breakdown of simulation time for the 10- and 20-component cases using the three different combinations of the algorithms. For example, use of the algorithms (CSA, FK) took 53% of the total simulation time on the phase-equilibrium calculations for the 10-component case and 66% for the 20-component case. **Table 4** also shows that use of (RSA, RF) resulted in phase-behavior calculations that were 63 and 85% faster than when (CSA, MG) and (CSA, FK) were used, respectively, for the 10-component case. For the 20-component case, the phase-behavior calculations using (RSA, RF) were 2.4 and 4.2 times faster than when (CSA, MG) and (CSA, FK) were used, respectively. The speed-up comes from the decreased calculation time using the Newton method (see **Table 4**), in which the reduced method exploits the reduced number of equations to be solved. **Fig. 6** shows the total simulation time for varying  $N_c$  and for different algorithms. Compared to the other algorithms, the reduced method offers more than 23 and 47% speed-up for the 10- and 20-component cases, respectively.

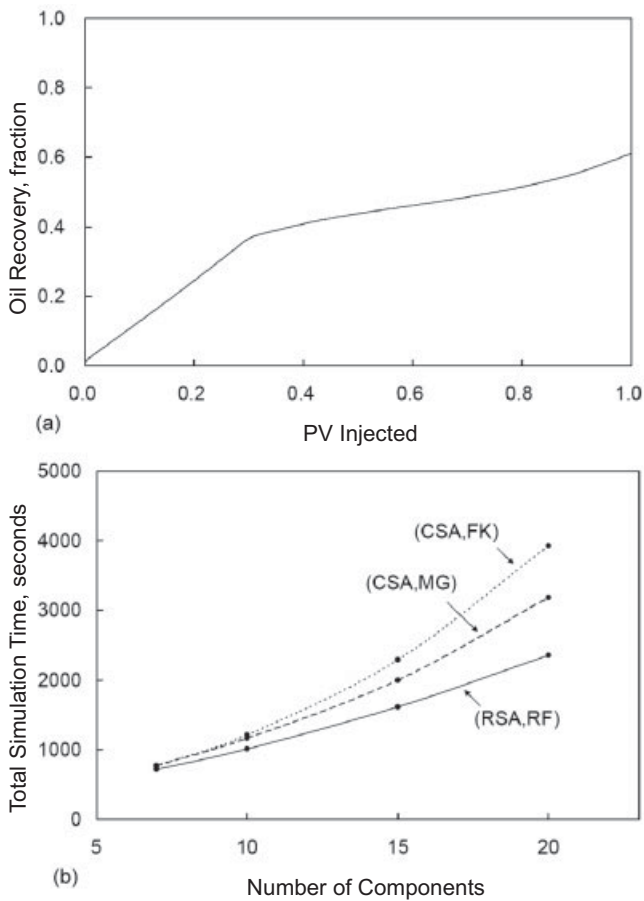
**Multicontact Miscible Case.** For this case, the initial, injection, and production pressures are set to 4,550, 4,600, and 4,100 psia, respectively. This case is more difficult for phase-equilibrium algorithms because the pressures are above the MMP and fluids are multicontact miscible. Location of a stationary point for stability analysis was performed approximately 1.3 million times, and flash calculations were performed approximately 2.3 million times. Average numbers of iterations for RSA, CSA, RF, MG, and FK were 1.9, 2.0, 1.3, 1.3, and 1.4, respectively. The RF converged to the trivial solution only four times, while the other two flash algorithms failed more than 20 times. Because of the increased failure rate with (CSA, MG) and (CSA, FK), the simulation results are not identical, although they are very similar (**Fig. 7**). The nonconvergence of MG and FK are consequences of the round-off errors caused by nearly singular Hessian and Jacobian matrices in the critical region (Trangenstein 1987). The four cases of a trivial solution with the RF occur where compositions are located in the vicinity of the binodal curves very near the critical region. In fact, liquid phase mole fractions of the correct solutions are  $L = 0.999, 0.997, 0.997,$  and  $0.998$ .

**Table 5** shows a breakdown of simulation time for 10- and 20-component cases using the three different combinations of the algorithms. When using the algorithms (CSA, FK), the phase equilibrium calculations spent 57% of the total simulation time for the 10-component case and 66% for the 20-component case. Also, use of (RSA, RF) resulted in the phase-behavior calculations that were 30 and 38% faster than when (CSA, MG) and (CSA, FK) were used, respectively, for the 10-component case. For the 20-component case, the phase-behavior calculations using (RSA, RF) were 1.8 and 2.5 times faster than when (CSA, MG) and (CSA, FK) were used, respectively. The speed-up is a consequence of the reduced number of equations to be solved in the Newton iteration using the reduced method (see **Table 5**). **Fig. 7** shows the total simulation times with different numbers of components and different algorithms. The use of the reduced method results in simulations that are more than 15 and 35% faster than those with

**TABLE 4—BREAKDOWN OF SIMULATION TIME FOR IMMISCIBLE CASE**

	10 components			20 components		
	(RSA, RF)	(CSA, MG)	(CSA, FK)	(RSA, RF)	(CSA, MG)	(CSA, FK)
Overall simulation (seconds)	123.6	152.6	164.6	296.0	435.7	612.7
Phase equilibrium (seconds)	47.5	77.3	87.7	96.6	236.3	406.0
Stability analysis, SS (seconds)	12.2	12.8	12.1	28.5	27.0	30.0
Stability analysis, Newton (seconds)	4.8	5.2	5.0	8.2	22.7	22.9
Flash calculations, SS (seconds)	9.5	9.7	9.3	21.3	22.0	21.3
Flash calculations, Newton (seconds)	21.1	49.7	61.3	38.6	164.5	331.9





**Fig. 7—Comparisons for the multicontact miscible case. (a) Oil recovery is identical for all algorithms. (b) Total simulation time vs.  $N_c$  for the different combinations of flash and stability algorithms.**

the other algorithms for 10- and 20-component cases, respectively. The speed-up factors of the total simulation time are smaller than for the immiscible case because part of the simulation time spent by the second-order convergence methods is smaller for this case. Similarly, if a larger number of grid cells is used, the speed-up factors will decrease because solution of the pressure equations takes a larger part of the total simulation time. Actual saved time, however, becomes more significant as the phase-equilibrium problems become more difficult and the simulation time becomes longer. For example, use of (RSA, RF) saved 1,574 seconds compared to (CSA, FK) for the multicontact miscible case and 317 seconds for the immiscible case. Also, the saved time would be even more significant if stability analysis for a single phase were performed for all cells, unlike in these case studies.

## Conclusions

A robust and efficient algorithm for two-phase equilibrium calculations using a reduced method was developed and implemented in a

compositional simulator. The simple algorithm exhibits improved convergence behavior near the critical region. Simulation case studies confirmed that the reduced method can significantly decrease compositional simulation time without loss of accuracy. Because of the significant speed-up, the use of the reduced method can allow for a larger number of components to be used in the simulation for improved accuracy of the fluid characterization.

## Nomenclature

- $A_i$  = EOS parameter for component  $i$
- $B_i$  = EOS parameter for component  $i$
- $f_i$  = fugacity for component  $i$
- $F_i$  = fugacity equation for component  $i$
- $F_j^R$  =  $j$ th equation for reduced flash calculations
- $g_i$  = parameter of component  $i$  for reduced method
- $h_i$  = parameter of component  $i$  for reduced method
- $k_{ij}$  = binary interaction coefficient between components  $i$  and  $j$
- $K_i$  =  $K$  value for component  $i$
- $L$  = liquid phase mole fraction
- $N_c$  = number of components
- $P_c$  = critical pressure
- $S_i$  = stationarity equation for component  $i$
- $S_k^R$  =  $k$ th equation for reduced stability analysis
- $T_c$  = critical temperature
- $V$  = vapor phase mole fraction
- $x_i$  = mole fraction of component  $i$  in a liquid phase
- $\underline{x}$  = vector with elements  $x_i$
- $X_i$  = independent variable for component  $i$  used for conventional stability analysis
- $y_i$  = mole fraction of component  $i$  in a vapor phase
- $z_i$  = mole fraction of component  $i$  in a mixture
- $\underline{z}$  = vector with elements  $z_i$
- $Z$  = compressibility factor
- $\varepsilon$  = stopping criteria for iterative solution
- $\eta_{ki}$  = constant term for component  $i$  to define  $k$ th reduced parameter
- $\theta_k$  =  $k$ th reduced parameter
- $\underline{\theta}$  = vector with elements  $\theta_k$
- $\varphi_i$  = fugacity coefficient for component  $i$
- $\psi_j$  =  $j$ th independent variables for reduced flash calculations
- $\underline{\psi}$  = vector with elements  $\psi_j$

## Superscripts

- $L$  = liquid phase
- $V$  = vapor phase
- $R$  = reduced method

## Subscripts

- $c$  = critical property or component
- $i$  = component index
- $j$  = component index, or index for variables or equations for reduced flash calculations
- $k$  = index for reduced parameters or for equations for reduced stability analysis

**TABLE 5—BREAKDOWN OF SIMULATION TIME FOR MULTICONTACT MISCIBLE CASE**

	10 components			20 components		
	(RSA, RF)	(CSA, MG)	(CSA, FK)	(RSA, RF)	(CSA, MG)	(CSA, FK)
Overall simulation (seconds)	1,010.8	1,164.2	1,214.1	2,352.2	3,186.3	3,926.5
Phase equilibrium (seconds)	498.6	645.9	690.3	1,051.1	1,867.4	2,588.6
Stability analysis, SS (seconds)	292.6	292.9	295.0	664.9	678.5	670.8
Stability analysis, Newton (seconds)	58.2	65.4	64.2	105.5	281.0	278.8
Flash calculations, SS (seconds)	32.9	34.3	34.2	74.7	77.1	73.0
Flash calculations, Newton (seconds)	114.9	253.2	296.9	205.9	830.8	1,566.0



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## Appendix A—Fugacity Coefficients Using Five Reduced Parameters

Fugacity coefficients at fixed temperature and pressure using the Peng-Robinson EOS (Peng and Robinson 1976) are as follows:

$$\begin{aligned} \ln \varphi_i(x) &= \frac{B_i}{B_m}(Z-1) - \ln(Z - B_m) \\ &\quad - \frac{A_m}{2\sqrt{2}B_m} \left( \frac{2\sum_{j=1}^{N_c} x_j A_{ij}}{A_m} - \frac{B_i}{B_m} \right) \ln \left[ \frac{Z + (1 + \sqrt{2})B_m}{Z + (1 - \sqrt{2})B_m} \right] \end{aligned}$$

for  $i = 1, \dots, N_c, \dots$  (A-1)

where

$$\begin{aligned} A_m &= \sum_{j=1}^{N_c} \sum_{l=1}^{N_c} x_j x_l A_{jl}, \\ B_m &= \sum_{j=1}^{N_c} x_j B_j, \end{aligned}$$

and

$$A_{ij} = \sqrt{A_i A_j} (1 - k_{ij}).$$

The fugacity coefficients are functions of five reduced parameters because  $A_m$ ,  $B_m$ ,  $Z$ , and  $\sum_j x_j A_{ij}$  can be expressed using those five reduced parameters. That is,

$$\begin{aligned} A_m &= \sum_{i=1}^{N_c} \sum_{j=1}^{N_c} x_i x_j \sqrt{A_i A_j} (1 - k_{ij}) \\ &= \sum_{i=1}^{N_c} \sum_{j=1}^{N_c} x_i x_j \sqrt{A_i A_j} \left[ 1 - (h_i - h_j)^2 g_i g_j \right] \\ &= \left( \sum_{i=1}^{N_c} x_i \sqrt{A_i} \right)^2 - 2 \left( \sum_{i=1}^{N_c} x_i \sqrt{A_i} h_i^2 g_i \right) \left( \sum_{i=1}^{N_c} x_i \sqrt{A_i} g_i \right) \\ &\quad + 2 \left( \sum_{i=1}^{N_c} x_i \sqrt{A_i} h_i g_i \right)^2 \\ &= \theta_2^2 - 2\theta_4 \theta_5 + 2\theta_3^2, \dots \dots \dots (A-2) \end{aligned}$$

$$B_m = \theta_1, \dots \dots \dots (A-3)$$

$$Z = Z(A_m, B_m) = Z(\theta_1, \theta_2, \theta_3, \theta_4, \theta_5), \dots \dots \dots (A-4)$$

and

$$\begin{aligned}
\sum_{j=1}^{N_c} x_j A_{ij} &= \sum_{j=1}^{N_c} x_j \sqrt{A_i A_j} (1 - k_{ij}) \\
&= \sum_{j=1}^{N_c} x_j \sqrt{A_i A_j} \left[ 1 - (h_i - h_j)^2 g_i g_j \right] \\
&= \sqrt{A_i} \sum_{j=1}^{N_c} x_j \sqrt{A_j} - \sqrt{A_i} h_i^2 g_i \sum_{j=1}^{N_c} x_j \sqrt{A_j} g_j \\
&\quad - \sqrt{A_i} g_i \sum_{j=1}^{N_c} x_j \sqrt{A_j} h_j^2 g_j \\
&\quad + 2\sqrt{A_i} h_i g_i \sum_{j=1}^{N_c} x_j \sqrt{A_j} h_j g_j \\
&= \sqrt{A_i} \theta_2 - \sqrt{A_i} h_i^2 g_i \theta_3 - \sqrt{A_i} g_i \theta_4 + 2\sqrt{A_i} h_i g_i \theta_3.
\end{aligned}$$

.....(A-5)

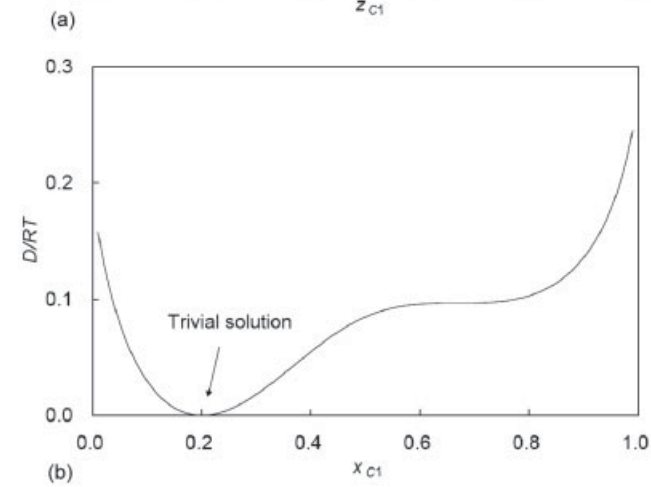
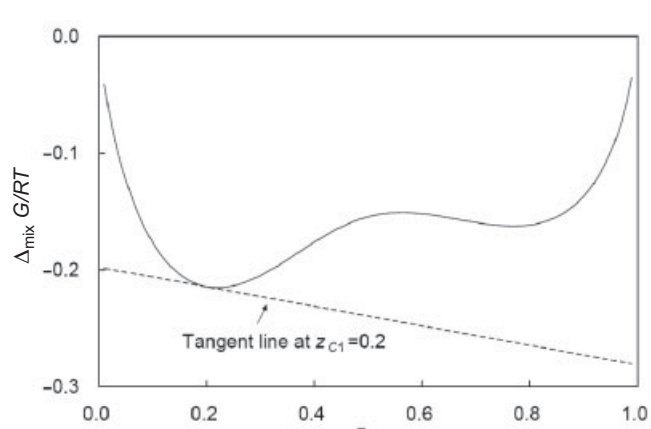
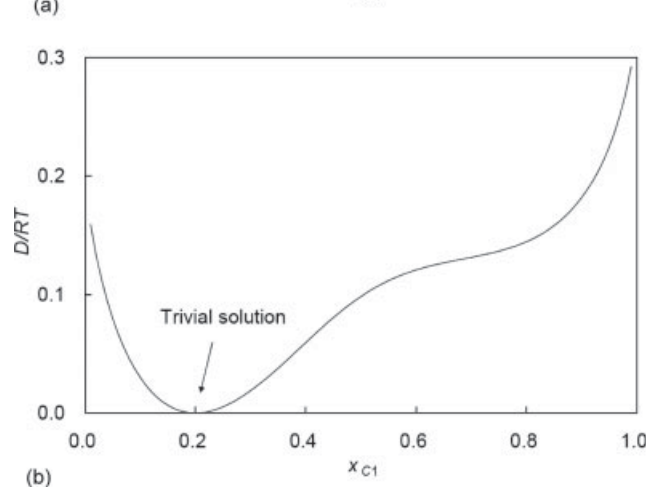
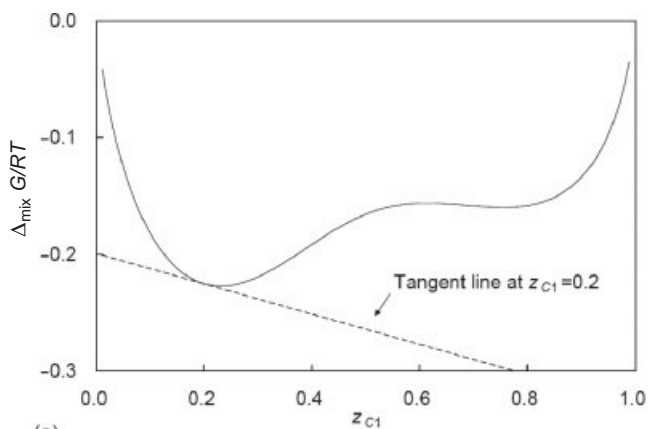
### Appendix B—Convergence Problem in the Region Slightly Outside the Shadow-Phase Region

We consider the stability analysis of a binary mixture consisting of 20%  $C_1$  and 80%  $n-C_{20}$ . The critical point of the mixture is calculated to be at 911.73°F and 312.63 psia using the Peng-Robinson EOS (Peng and Robinson 1976). **Figs. B-1, B-2, and B-3** show construction of the dimensionless TPD function ( $D/RT$ ) at a fixed temperature of 800°F and three different pressures of 690, 633, and 575 psia, respectively. Those pressures are in the single-phase region in the P-T diagram because  $D/RT$  is nonnegative in the entire  $x_{c1}$  space. The outer boundary of the shadow-phase region at this temperature is at 632.7 psia, where a saddle point exists on the TPD function. For the case of 690 psia,  $D/RT$  has a unique minimum that corresponds to the trivial solution. For the case of 633 psia,  $D/RT$  also has the same unique minimum. However, the gradient becomes very close to zero at the inflection point around at  $x_{c1} = 0.67$ . For the

case of 575 psia,  $D/RT$  has two minima; one is the trivial solution, and the other is a nontrivial solution with a positive value of  $D/RT$ . When a local-minimization algorithm is used with a vapor-like initial estimate, the algorithm obtains the local minimum at  $x_{c1} = 0.76$ . Therefore, when the local minimum of  $D/RT$  converges by using a vapor-like estimate as the initial guess is plotted as a function of pressure, there exists a discontinuity at 632.7 psia, the outer boundary of the shadow-phase region (**Fig. B-4**). This discontinuity is what Hoteit and Firoozabadi (2006) reported in their paper for different mixtures. The global minimum should not exhibit this kind of discontinuity because the global minimum of  $D/RT$  should be always zero in a single-phase region.

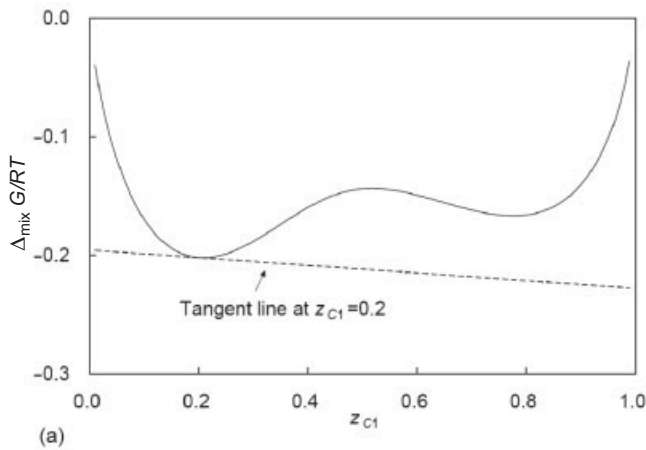
When the conditions are closer to the critical point, the location of the saddle point becomes closer to the trivial solution and the degree of discontinuity becomes smaller. **Fig. B-5** shows  $D/RT$  at a temperature of 900°F and a pressure of 377 psia. The outer boundary of the shadow-phase region at this temperature is at 376.5 psia. When stability analysis is performed for this mixture with a vapor-like initial estimate, the improved RSA and CSA require 21 and 33 iterations to decrease  $\max\{|S_j|\}$  from  $10^{-3}$  to  $10^{-10}$ , respectively. The poor convergence behaviors arise from the existence of the inflection point with a very small value of the gradient because it tends to attract the values for each subsequent iteration.

There are several approaches to improve the problem. The safest approach would be to take a larger number of SS steps to provide a better initial estimate for the Newton method. Another approach is to use a global minimization algorithm for the TPD function. However, those time-consuming methods would not be justified to use in compositional simulation because the standard stability analysis using the stationary point method assumes a stable single-phase when convergence cannot be achieved within a specified number of iterations. Therefore, a practical approach

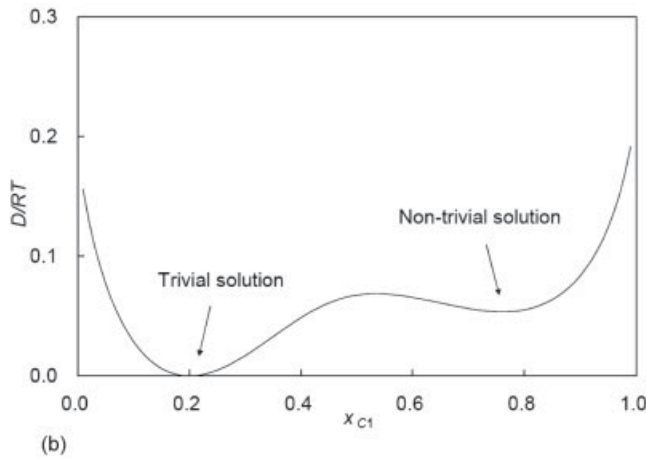


**Fig. B-1—Construction of the TPD function for a mixture of 20%  $C_1$  and 80%  $n-C_{20}$  at 800°F and 690 psia. (a) The dimensionless molar Gibbs free energy of mixing. (b) The dimensionless TPD function.**

**Fig. B-2—Construction of the TPD function for a mixture of 20%  $C_1$  and 80%  $n-C_{20}$  at 800°F and 633 psia. (a) The dimensionless molar Gibbs free energy of mixing. (b) The dimensionless TPD function.**



(a)



(b)

**Fig. B-3—Construction of the TPD function for a mixture of 20% C<sub>1</sub> and 80% n-C<sub>20</sub> at 800°F and 575 psia. (a) The dimensionless molar Gibbs free energy of mixing. (b) The dimensionless TPD function.**

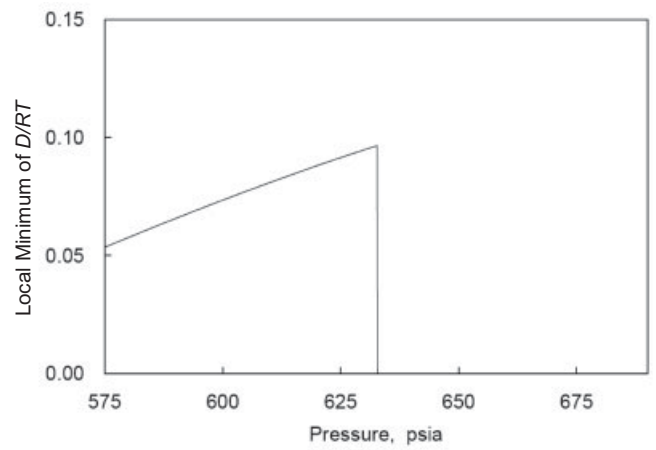
for compositional simulation would be simply to stop the iteration and assume a stable single phase when the iterations do not sufficiently improve the objective function for a few consecutive iterations (e.g., five iterations). The procedure of Hoteit and Firoozabadi (2006) would be another practical approach. They set the maximum number of iterations to be 15 for the reduced method, and they assume a stable single phase when convergence cannot be achieved within the maximum number of iterations.

### SI Metric Conversion Factors

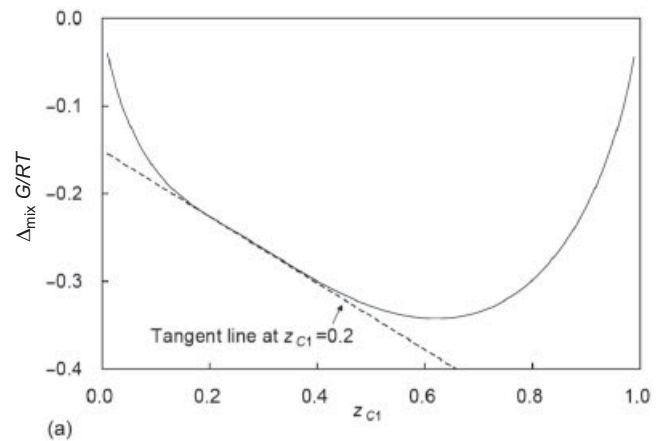
cp × 1.0*	E-03 = Pa·s
ft × 3.048	E-01 = m
°F (°F-32)/1.8	= °C
psi × 6.894757	E+00 = kPa

\*Conversion factor is exact.

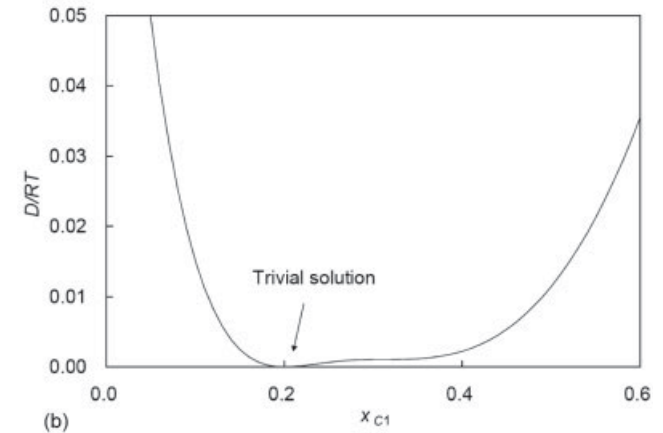
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**Fig. B-4—Local minimum of D/RT for a mixture of 20% C<sub>1</sub> and 80% n-C<sub>20</sub> at 800°F converged by starting with a vapor-like initial estimate. There is a discontinuity at 632.7 psia corresponding to the outer boundary of the “shadow-phase region.”**



(a)



(b)

**Fig. B-5—Construction of the TPD function for a mixture of 20% C<sub>1</sub> and 80% n-C<sub>20</sub> at 900°F and 377 psia. (a) The dimensionless molar Gibbs free energy of mixing. (b) The dimensionless TPD function.**

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