Compositional Space Parametrization for Miscible Displacement Simulation

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Abstract. Thermodynamic equilibrium computations are the most time consuming part of a compositional flow simulation. We describe a compositional space parameterization approach for dealing with gas injection displacement processes. This tie-line based parameterization can be used to replace existing compositional simulation methods completely. We illustrate our approach using numerical examples of challenging multi-component miscible gas injection problems.

1. Introduction

Compositional formulations of flow and transport in porous media are used to model miscible gas injection processes for enhanced oil recovery. In these processes accurate description of components transfer between multiple fluid phases is necessary. Compositional reservoir simulators usually employ an Equation of State (EOS) model to describe the phase behavior of these complex mixtures (Coats, 1980)-(Aziz and Wong, 1988).

For each cell, or control volume, in the computational domain, given the temperature, pressure, and overall composition of each component in the mixture, EOS computations are used to first determine the phase-state of the mixture (i.e., single-phase gas, single-phase liquid, or two phases), and if a two-phase state is indicated, flash calculations are used to obtain the equilibrium phase compositions (Michelsen, 1982; Firoozabadi, 1999). These two types of EOS calculations, namely, the phase state identification and flash calculations, are time consuming. Significant research efforts aimed at improving both the robustness and computational efficiency of compositional flow simulation are ongoing. Important challenges include: (1) the phase behavior of mixtures with large numbers of components in the critical region, (2) three-phase flash calculations, and (3) large-scale simulation of thermal-compositional displacement processes.

The computational cost of compositional flow simulation increases dramatically with the number of components used to represent the (hydrocarbon) fluid system. As a result, it is common practice to use lumping procedures to represent the thermodynamic behavior using a small

set of pseudo components. There have been several attempts to describe near-miscible gas injection recovery processes using pseudo-ternary representations (Helfferich, 1981)-(Barenblatt et al., 1990). Many investigators proposed that such ternary representations may be applicable for general multi-component problems.

In the 1990's, Orr and his research group (Monroe et al., 1990)-(Dindoruk et al., 1993) performed experimental and theoretical studies of gas injection processes for enhanced oil recovery. They presented a unified Method of Characteristics (MOC) theory of one-dimensional, multi-contact miscible gas-injection processes for mixtures with large numbers of components. In this theory, the solution path in compositional space is described using tie-lines. For a particular pressure and temperature, a tie-line connects compositions at either end of the two-phase envelope, which are the equilibrium compositions associated with any overall composition along the tie-line; moreover, compositional variation along a tie-line are consistent with the component mass-balance equations. The MOC based analytical theory revealed a complex set of behaviors and has led to fundamental contributions to our understanding of the physics associated with compositional displacement processes. In essence, that body of work (Orr, 2006) indicates clearly that the structure and properties of the tie-line space dictate the solution route in compositional space for gas injection processes. Moreover, that work indicates clearly that displacements involving more than three components can yield significantly different flow behaviors than those associated with pseudo-ternary models.

Based on the ideas of Orr et al. (Monroe et al., 1990)-(Dindoruk et al., 1993), an alternative approach to compositional flow simulation was developed (Entov, 1997)-(Voskov, 2002). In that approach, the description of gas injection processes is simplified using a parametrization of the compositional space based on tie-lines. A similar approach was suggested by Bedrikovetsky et al. (Bedrikovetsky and Chumak, 1992) for systems with constant partitioning coefficients. Here, we present a compositional space parametrization framework for speeding up the EOS computations associated with large-scale compositional flow simulations, where a large number of components is used. The methodology is based on combining two parameterizations with standard compositional formulations. The first is a tie-line based parameterization of the compositional space, which is valid within the region of tie-line extensions. The second is a parameterization of the critical tie-line surface, which is used to decide if a composition is in the supercritical state.

We present a tie-line based parameterization of the compositional space, including an adaptive strategy, where only the necessary tie-lines

are computed and tabulated. We then describe a robust and efficient approach for the parametrization of the critical tie-line surface. The two parameterizations are combined in order to speed up the EOS computations associated with compositional simulation. The overall methodology was implemented in a general purpose research simulator. We demonstrate the robustness and computational efficiency of the parameterization framework using several challenging multi-component gas injection problems. The summary and conclusions are given in the last section.

2. Compositional Space Parameterization (CSP)

Consider a system of n_c components and n_p fluid phases. Assume that a hydrocarbon component can exist in two hydrocarbons phases. The overall mole fraction of a component in the mixture, z_i, can be written as

$$z_i = x_i L + y_i(1 - L), \quad i = 1, \ldots, n_h, \tag{1}$$

where x_i and y_i denote the mole fraction of component i in the liquid and gas phases, respectively, and L is the volume fraction occupied by liquid phase. Using one of the components, say the first one, we can write

$$L = \frac{z_1 - y_1}{x_1 - y_1}. \tag{2}$$

The Compositional Space Parameterization (CSP) method is based on using the structure and properties of the tie-line space to parameterize the compositional space. This is possible because along a tie-line, or its extension, the overall concentration and fractional flow of a component can be written as a linear function of the tie-line parameters and the concentration of one of the components (say the first) (Entov, 1997). To show this, we substitute Eq. (2) into Eq. (1), which leads to

$$z_i = A_i z_1 + B_i, \quad i = 2, \ldots, n_h, \tag{3}$$

where

$$A_i = \frac{x_i - y_i}{x_1 - y_1}, \quad B_i = y_i - y_1 \frac{x_i - y_i}{x_1 - y_1}. \tag{4}$$

Equations (3)-(4) indicate that the overall composition of any component can be expressed as a linear function of the overall composition of the first component; the parameters A_i and B_i are constants for a

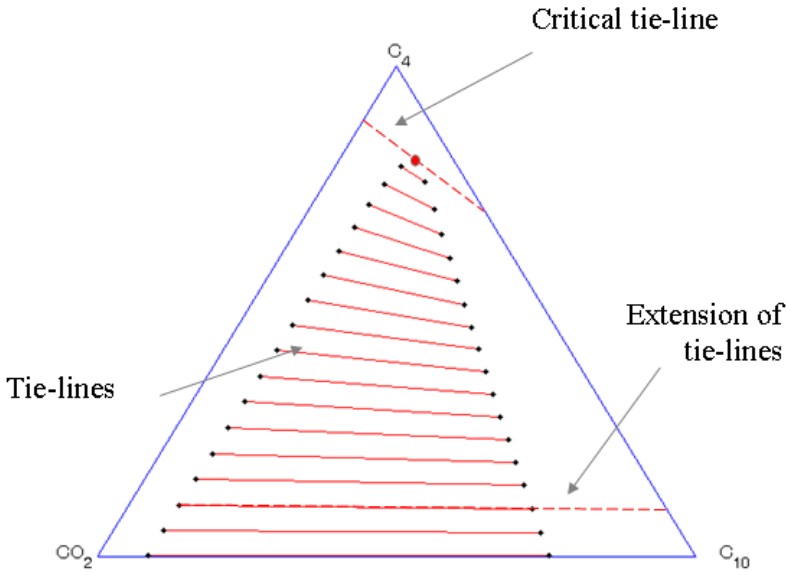


Figure 1. Ternary diagram for system $\{CO_2, C_4, C_{10}\}$ at $p = 800$ psi, $T = 400^o$ F

given tie-line in the two-phase region, or its extension, (see Fig.1), and they change only when we change tie-lines.

We replace the composition vector $\mathbf{z}, \{z_i, i = 1 \dots n_c\}$ with a new set of independent variables, namely, z_1 and $\gamma = \{\gamma_i, i = 1 \dots n_c - 1\}$. The vector γ is constant for a particular tie-line. Thus, for an arbitrary number s of tie-lines that cover the compositional space, z_1 and γ vectors can be used to define the compositional space completely. The quantities x_1, y_1, A_i and B_i are easily written in terms of γ. The thermodynamic behavior of these quantities in Γ-space can be described using polynomial approximations, for example (Entov et al., 2001; Voskov, 2002).

Notice that the definition in (4) means that for cases when x_1 is close to y_1, solutions of (3) may be difficult. This conditions occurs (1) when we are close to the plane $z_1 \equiv 0$, or (2) when we are close to the critical region. In the first case, one can switch to a different primary component. This can be easily performed based on $\{z_i\}$ distribution. For the second case, several approaches for dealing with compositions in the super-critical region may be used. A discussion of this is provided later.

Parameterization of the tie-line space using the new variable set allows the splitting of the overall compositional displacement problem

into thermodynamic and hydrodynamic parts. Consider the system of conservation laws for 1D incompressible two-phase flow in porous media

$$m\frac{\partial z_i}{\partial t} + U\frac{\partial F_i}{\partial x} = 0, \quad i = 1, \ldots, n_c - 1, \tag{5}$$

where F_i is the overall fractional flow of component i defined as $F_i = x_i F(s) + y_i(1 - F(s))$, and $F(s)$ is the fractional flow of the liquid phase. Using the parameterization in terms of z_1 and γ, the system of equations (5) can be written as follows:

$$m\frac{\partial z_1}{\partial t} + U\frac{\partial F_1}{\partial x} = 0, \tag{6}$$

$$m\frac{\partial A_i(\gamma)z_1 + B_i(\gamma)}{\partial t} + U\frac{\partial A_i(\gamma)F_1 + B_i(\gamma)}{\partial x} = 0, \quad i = 1, \ldots, n_c - 2. \tag{7}$$

To simplify the description, we take $U/m = 1$.

A splitting procedure is used to solve (6)-(7) with appropriate initial and boundary conditions (Entov, 1997; Entov, 1999). The overall problem is decomposed into a hydrodynamic part, which is cast in terms of the parameterized compositional space, and a thermodynamic part. The (auxiliary) thermodynamic problem is formulated in terms of the tie-line parameters A_i and B_i, namely,

$$\frac{\partial A_i(\gamma)}{\partial t} + \frac{\partial B_i(\gamma)}{\partial y} = 0, \quad i = 1, \ldots, n_c - 2, \tag{8}$$

Notice that A_i and B_i are only functions of γ. Thus, the solution of this problem (8) depends only on the thermodynamic behavior of the system and is independent of hydrodynamic effects.

The second part deals with the hydrodynamic problem, which can be expressed using the following two equations

$$\frac{\partial z_1}{\partial t} + \frac{\partial F_1}{\partial x} = 0, \tag{9}$$

$$\frac{\partial A_j(\gamma(\sigma))z_1 + B_j(\gamma(\sigma))}{\partial t} + \frac{\partial A_j(\gamma(\sigma))F_1 + B_j(\gamma(\sigma))}{\partial x} = 0. \tag{10}$$

In these equations, the variation of γ along a tie-line (Γ) space is assumed to be a known function of the scalar parameter σ, which varies monotonically along the solution path.

It can be shown that projection of stable waves and shocks in (standard) compositional space, which form the solution of (6)-(7) for incompressible one-dimensional problems, into Γ-space corresponds to stable waves and shocks in the solution of the thermodynamic problem (Entov,

1997). Moreover, the solution path in Γ-space is independent of the hydrodynamic properties (e.g., relative permeability, viscosity, density) of the initial system and depends only on the thermodynamics properties (e.g., initial/injection compositions). For one-dimensional problems, invariance of the solution path in Γ-space with respect to variations in the hydrodynamic variables was shown also for compressible flows with density variation (Entov et al., 2001; Voskov, 2002).

The method just described was implemented in an alternative multi-dimensional compositional simulator (Entov et al., 2001; Voskov, 2002), where polynomial interpolation was used to parameterize the tie-line space. For studies with significant changes in pressure, the polynomial coefficients were linearly approximated as a function of pressure.

3. Phase Behavior Using Compositional Space Parameterization

To simplify the description, we take the temperature T to be constant. For each pressure in the interval of interest, we construct the phase diagram using a fixed density of tie-lines (Entov et al., 2001; Voskov, 2002). All the calculated tie-lines are stored in a table.

To represent a tie-line as function of γ, we use natural neighbor interpolation (Sibson, 1981) where the tie-line space is discretized using a Delaunay triangulation. For any tessellation of un-scattered data, interpolation of any point inside hyper-triangle is performed

$$\lambda_i = \sum_{k=1}^{n} a_{i,k}\gamma_k + b_i, \quad i = 1, \ldots, n+1 \tag{11}$$

where λ_i denote the barycenter coordinates of each neighbor ($n+1$ neighbor for n-dimension space), γ_k is the coordinate of the interpolated point in the k direction. In order to find coefficients $a_{i,k}$ and b_i, we use the barycenter coordinate, which serves as a basis vector for each vertex.

Thus, we can write a system of equations for each vertex

$$e_i = \Gamma a_i + b_i, \quad \forall i \in 1, \ldots, n+1 \tag{12}$$

Here Γ is a matrix of the coordinates of all the neighbors ($n+1 \times n$), and e_i is a unit vector ($e_1 = [1, 0, \ldots, 0]$, $e_2 = [0, 1, 0, \ldots, 0]$, etc.). In order to find coefficients a_i and b_i, we solve (12) for each e_i. That is, we compute the inverse of matrix $[\Gamma \quad 1]$.

Inside a hyper-triangle, linear interpolation is used. For that purpose, we find the exact solution of following general problem

$$L = \frac{z_m - y_m}{x_m - y_m}, \quad \forall m \in [1, \ldots, n_c - 1], \tag{13}$$

$$f_j = x_j L + y_j(1 - L) - z_j = 0, \quad j = 1, \ldots, n_c - 1. \tag{14}$$

For the tie-line space, we have following correspondence between n from (11) and n_c: $n = n_c - 2$.

Using (11), we can write the following linear system of equations

$$\sum_{i=1}^{n+1} f_{ij} \left(\sum_{k=1}^{n} a_{i,k} \gamma_k \right) = - \sum_{i=1}^{n+1} f_{ij} b_i, \quad j = 1, \ldots, n \tag{15}$$

or in matrix representation

$$\mathbf{fA}\gamma = -\mathbf{fb}. \tag{16}$$

The solution of this system, γ, provides the barycenter coordinates for the interpolation of x_j and y_j, which corresponds to the flash results of the composition of interest. This solution is performed for the pre-calculated tie-line set for pressure points p^k and p^{k+1}. Linear interpolation is used to compute the phase fractions for a pressure $p \in [p^k, p^{k+1}]$. In Fig. 2, you can see corresponding tie-lines that are involved in the solution of (13)-(14) for both pressures $p^k = 2300$ and $p^{k+1} = 3000$.

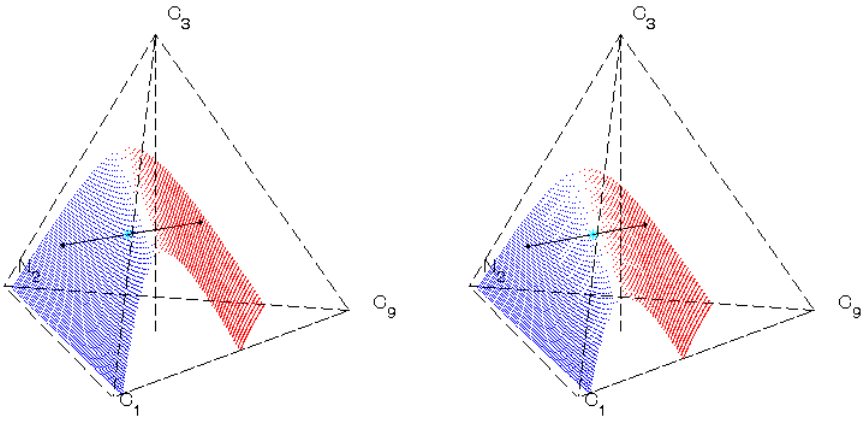


Figure 2. Tetrahedral diagrams for four-component $\{N_2, C_1, C_3, C_9\}$ system at $p = 2300$ (left) and $p = 3000$ psi (right) for $T = 270^o$ F and randomly generated composition $\{0.42, 0.10, 0.27, 0.21\}$ with corresponding tie-lines.

This procedure was tested for the wide range of multi-component systems using randomly generated compositions. The largest error for

the CSP-based flash calculations was always less than 1%, which is within the precision of EOS-based flash computations when compared to experimental observations. To demonstrate robustness of the CSP-based table look-up approach, several numerical experiments were also performed. One-dimensional gas injection problems for several hydrocarbon systems were solved using a variety of injection and initial compositions. We assume that the overall compressibility is low and that the dependence of composition on pressure differences is small.

Here, we present results for a problem where a gas composed of $\{CO_2(80\%), C_1(20\%)\}$ is injected into a homogeneous reservoir containing oil $\{CO_2(5\%),\ C_1(20\%),\ C_4(30\%),\ C_{10}(45\%)\}$. For flash calculations, two table look-up schemes were implemented. The first method take the closest calculated tie-line from the table in order to minimize the norm of (14). These solutions are shown in Fig. 3 as the green dashed line. In the second method, Delaunay triangulation of the parameterized compositional space is performed, and the problem (13)-(14) is solved. The solution calculated using this method is shown in Fig. 3 as the red dotted line. Simple Corey relative permeability curves and constant viscosities were used in the calculations. In Fig. 3, the two CSP-based solutions are compared with standard EOS simulation results (blue solid line). Some differences between the solutions are present, and they are due to ignoring compressibility effects in the CSP-based table look-up methods.

It is possible to improve the performance of these methods using localization procedures. The properties of the solution path in Γ-space can be used to localize the search space. One way to speed up the procedure is to use a dynamic table look-up strategy, where the relevant tie-lines are stored in the course of simulation. A tie-line appears in the table only if it is part of the solution path in Γ-space. As a result, the number of stored tie-lines in the table is usually a very small subset of all the tie-lines in the compositional space. The optimization procedure begins by looking through the table. If the solution with the required tolerance is not in the table, the optimization procedure switches to a complete table of the parameterized compositional space. The tie-lines involved into interpolation are copied from the complete table to the dynamic table.

In practice, it is common to run sensitivity analysis for a large number of problems with different reservoir description models, or with slightly different injection compositions. In these cases, the CSP-based table constructed from a previous compositional simulation can be used as the starting point for the next run, and this can lead to great savings in the overall computational cost of performing a simulation study.

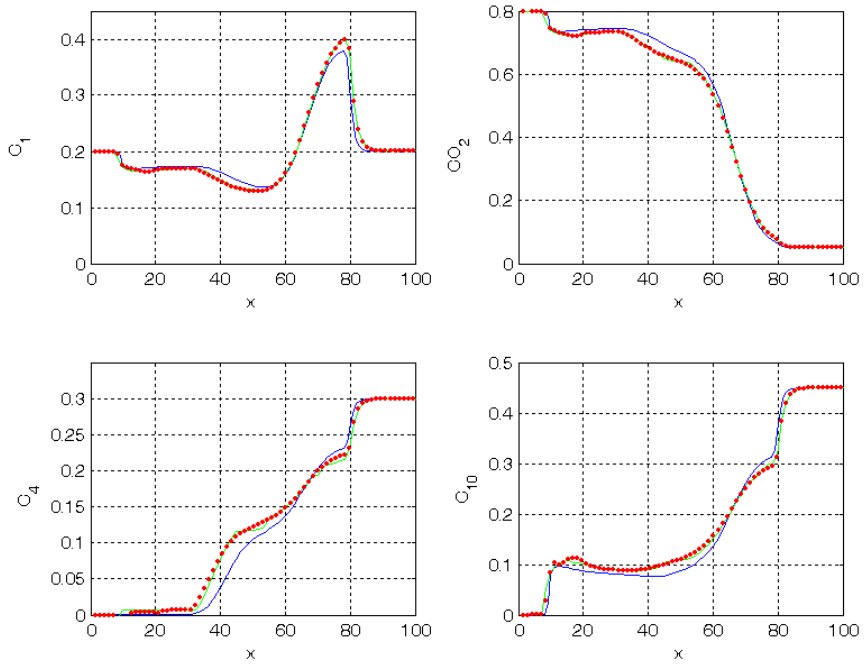


Figure 3. Solution of gas injection problem into oil made up of $\{CO_2, C_1, C_4, C_{10}\}$. Dashed and dotted lines - table look-up flash, solid line - eclipse solution.

Fig. 4 shows the frequency of tie-lines used during the simulation of gas injection cases shown in Fig. 3. Quadratic relative permeability functions for the full (red) and partial (green) simulation runs are shown. Simulations using cubic relative permeability functions are also presented (blue). All the data were sorted based on the frequency of the red points. Examination of the figure indicates that a limited number of tie-lines is used (about 3% of the total set of tie-lines covering the compositional space), and the used tie-lines tend to be the same for the different cases. Moreover, during a simulation run the tie-line set is fixed, but the frequency of usage increases. This is consistent with previous observations that the solutions in tie-line space are largely invariant with respect to the hydrodynamic properties (Voskov, 2002; Voskov and Tchelepi, 2007).

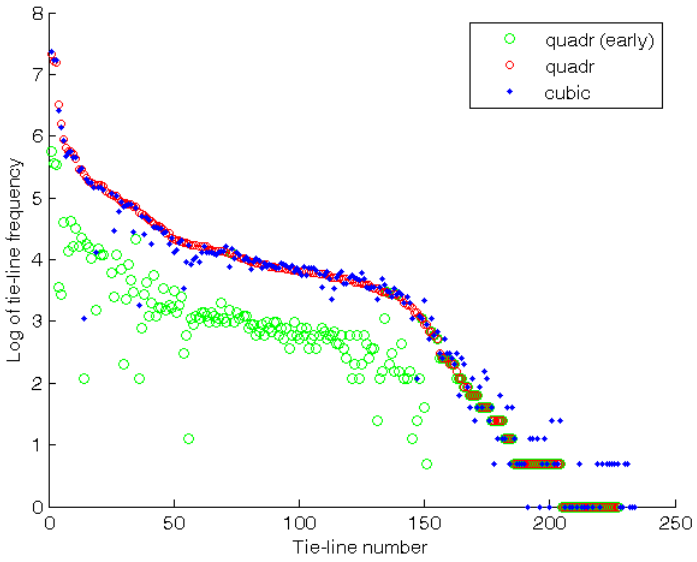


Figure 4. Solution of gas injection problem presented on Fig. 3 with different relative permeabilities. Green and red frequency are taken for different time steps (earlier and later respectively).

4. Compositional Space Adaptive Tabulation (CSAT)

One can construct the tie-line parametrization as a pre-processing step. Then, the CSP approach can be used to replace standard EOS computations in reservoir flow simulation, including the phase stability test and the flash calculations. In that case, however, a large number of tie-lines may be needed. In this section, we describe an adaptive strategy where we compute the necessary tie-lines only.

For gas injection processes, the solution route in compositional space can be split into two types: (1) tie-line paths, which connect points along a fixed tie-line (or its extension), and (2) non tie-line paths, where points on different tie-lines are connected (Orr, 2006). Thus, a limited number of 'key' tie-lines are involved in the solution route. In practice, it is often the case that a single-phase gas mixture is injected to displace the resident hydrocarbon liquid. If the initial and injected compositions remain fixed during the displacement process, the solution route involves these two tie-lines (see Fig. 5).

For the particular displacement problem of interest, we specify a set of compositions and a pressure range. The composition set is chosen using information about the likely key tie-lines. The tie-lines associated with the initial and injection composition are obvious candidates. A

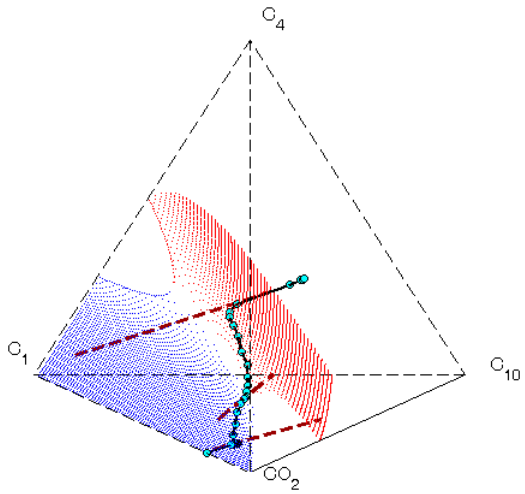


Figure 5. Solution of gas injection problem for composition $\{CO_2\,,\ C_1\,,\ C_4\,,\ C_{10}\}$ in compositional space. In dashed brown lines initial, injection and intermediate tie-lines are shown.

table is constructed where for each composition in the specified set, the tie-lines corresponding to each pressure value in the interval of interest are computed and stored.

During a simulation run, whenever a phase stability test, or flash, is needed, we check if the composition lies on one of the stored tie-line. To check the composition, we use a modification of (1)-(2)

$$L = \frac{z_j - y_j}{x_j - y_j} \tag{17}$$

$$\sum_{i=1}^{n_c} \left(x_i L + y_i(1-L) - z_i\right)^2 < \varepsilon. \tag{18}$$

If one of the stored tie-lines satisfies these criteria for the composition, the table is used to look up the flash (phase compositions) results. Otherwise, a standard EOS based phase behavior procedure is employed. In this strategy, which we refer to as Compositional Space Tabulation (CST), we work with the fixed table of tie-lines; a composition that is not intersected by one of the original key tie-lines, is dealt with using a standard EOS scheme.

The result of the CST implementation for test cases (see Table I) demonstrate that this preconditioning can lead to a several-fold speed up of compositional flow simulation. Using a simple and computationally inexpensive check (17)-(18), the compositional space parametriza-

tion replaces the time consuming phase-stability iterations associated with standard compositional simulation methods.

We are interested in speeding up compositional modeling of practical multi-dimensional problems, where the compositional solutions are accompanied with a certain amount of dispersion. In these cases, the solution path may involve not only the key tie-lines, but also several neighboring tie-lines. In order to include these tie-lines into the simple CSP-based checking procedure, a Compositional Space Adaptive Tabulation (CSAT) approach is employed.

Each time a phase-state stability test is required in a compositional simulation, we check the set of stored tie-lines. If the composition does not lie on any of the stored tie-lines, new tie-lines are computed for the pressure range of interest. Both the CST and CSAT methods were implemented in a General Purpose Research Simulator (GPRS) (Cao, 2002).

We note that Pope (Pope, 1997) proposed the In Situ Adaptive tabulation (ISAT) method for modeling turbulent reactive combustion. Our CSAT approach uses a similar idea, where the compositional space is tabulated and adaptively updated. However, the specifics of the problem, the governing mathematical statement, and the parametrization framework are completely different.

We present two standard examples to demonstrate effectiveness of Compositional Space Tabulation procedures.

- Modification of SPE 3 test case (Kenyon and Behie, 1983): injection of a two-phase mixture composed of $\{N_2\ (80\%), C_1\ (10\%), C2\ (10\%)\}$ into oil made up of $\{CO_2\ (1.2\%),\ N_2\ (1.9\%),\ C_1\ (16\%),\ C_2\ (8.7\%),\ C_3\ (5.9\%),\ C_{4-6}\ (9.7\%),\ C_{7+1}\ (4.7\%),\ C_{7+2}\ (11.5\%),\ C_{7+3}\ (40.3\%)\}$. A 5-spot pattern, discretized using $50 \times 50 \times 5$ gridblocks, is used.

- The SPE 5 WAG injection problem (Killough and Kossack, 1987): the reservoir model is made up of $7 \times 7 \times 3$ gridblocks. Gas is composed of $\{C_1\ (77\%),\ C_3\ (20\%),\ C_6\ (3\%)\}$. The oil composition is $\{C_1\ (50\%),\ C_3\ (3\%),\ C_6\ (7\%),\ C_{10}\ (20\%),\ C_{15}\ (15\%)\},\ C_{20}\ (5\%)\}$. The injected gas is miscible with the resident oil for the pressure interval of interest.

- SPE 5G: modification of the SPE 5 problem. Injection of the pure methane C_1 into oil composed of $\{C_1\ (30\%),\ C_3\ (3\%),\ C_6\ (7\%),\ C_{10}\ (20\%),\ C_{15}\ (40\%)\}$. The injected gas is immiscible with the resident oil for the pressure interval of interest.

Table I present results obtained using the Composition Space Tabulation (CST) and the Compositional Space Adaptive Tabulation (CSAT)

Table I. Comparison for standard, CST, and CSAT compositional simulations

Test	Type of EOS	Stab. it., 10^3	Checks, 10^3	Tie-lines	EOS time
SPE 3	standard	95071 + 19873	–	–	1674
	CST	15620 + 3678	11762	2	323
	CSAT (10^{-3})	134 + 38	14806	19	52
	CSAT (10^{-4})	77 + 23	28463	101	50
SPE 5	standard	15001 + 1490	–	–	101
	CST	7956 + 581	227	1	52
	CSAT (10^{-3})	4678 + 206	448	3	18
	CSAT (10^{-4})	5320 + 271	723	7	16
SPE 5	original	9309	–	–	35
mod	CST	41	404	2	1
	CSAT ($\varepsilon = 10^{-3}$)	9	398	1	< 1
	CSAT ($\varepsilon = 10^{-4}$)	8	402	2	< 1

procedures. CSAT was run with different precision (ε from (18)). The stability iteration count includes phase stability tests, flash calculations, and surface-condition flashes (both SSI and Newton). The Table also shows the number of tie-line checks performed. The phase behavior time (in seconds) includes the time spent on stability tests, flash calculations, and checking procedures (both tie-line look-up and computation of new tie-lines as needed by CSAT).

More extended testing, including sensitivity test can be found in (Voskov and Tchelepi, 2007). Analysis of the results in the Table I indicates that the CSAT method is not very effective when one of the compositions is in the super-critical region (injection composition in SPE 5). In the next section we are going to present numerically effective procedure for detecting such condition.

5. Supercritical State Criteria (SSC) method

Miscible and near-miscible compositional displacements of practical interest often require accurate description of the phase behavior in the critical region. This poses a significant challenge to the CSP approach since tie-lines are not defined beyond the critical region; as a result, compositions beyond the region of tie-line extensions (i.e., supercritical region) cannot be parameterized using tie-lines. For problems where

the solution path involve the supercritical region, we combine the tie-line based parameterization framework with conventional approaches to cover the full compositional space. For that purpose, we need to present robust and efficient procedures for detecting that a composition lies in the supercritical region. The idea is to parameterize the critical tie-line surface itself.

The tie-line calculation algorithm is based on using pseudo-ternary slices of the compositional diagram, starting with longest tie-line (Entov et al., 2001; Voskov, 2002). This procedure continues using successive pseudo-ternary slices until a single-phase state is detected. This approach ensures that the last computed tie-line is close to critical one, with a predefined tolerance. The first step of the approach is to collect all the critical tie-lines.

Next we need to determine if a composition is supercritical. Geometrically, this corresponds to identifying if a point in multi-dimensional space is above or below the critical tie-line surface (see Fig. 6).

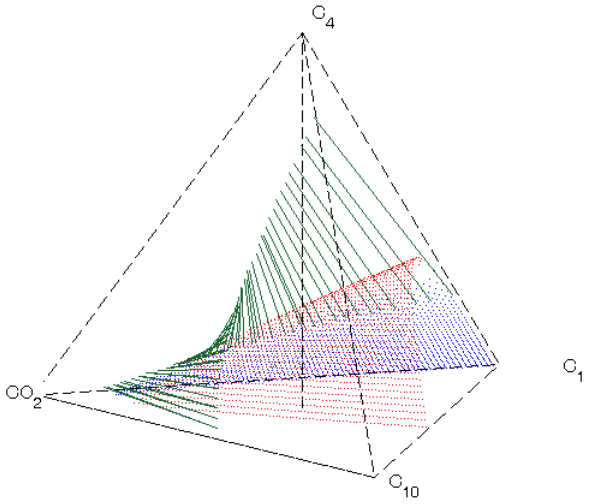


Figure 6. Critical subsurface for the system $\{CO_2, C_1, C_4, C_{10}\}$ at $p = 2300$ psi.

For a composition that belongs to the critical tie-line surface, we can write the following equation

$$z_i^c = Lx_i^c + (1 - L)y_i^c, \quad i = 1, \ldots, n_c \tag{19}$$

It is obvious that for any critical point we have $x_i^c = y_i^c$. Numerically, we can parameterize the critical surface by using the criteria $0 < |x_i^c - y_i^c| < \varepsilon$. Notice also that parameter L can vary as $-\infty < L < \infty$.

For any critical tie-line, we need to find the distance from the given composition $\mathbf{Z}$ (red point on Fig. 7) to a point on the critical surface $\mathbf{z^c}$ (blue point on Fig. 7). That can be written as an optimization problem as follows

$$\min F(L) = \sum_i (z_i^c - Z_i)^2 = \sum_i (Lx_i^c + (1-L)y_i^c - Z_i)^2. \tag{20}$$

Using the criteria for minima of a function, we can obtain

$$\frac{\partial F}{\partial L} = \sum_i 2(Lx_i^c + (1-L)y_i^c - Z_i)(x_i^c - y_i^c) = 0, \tag{21}$$

which we use to define the value for L as

$$L = \frac{\sum_i (Z_i - y_i^c)(x_i^c - y_i^c)}{\sum_i (x_i^c - y_i^c)^2} \tag{22}$$

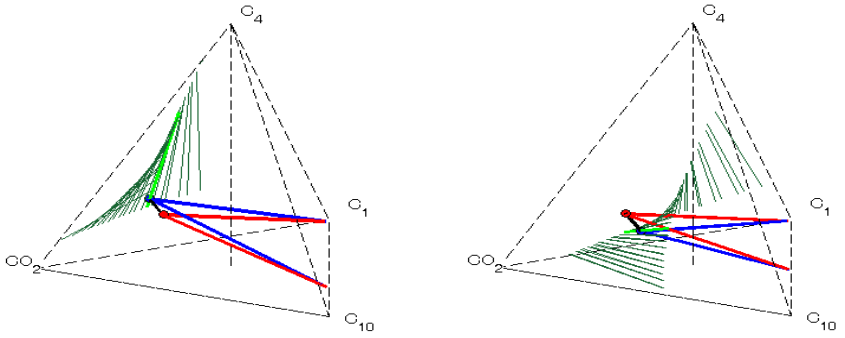


Figure 7. Checking the supercritical criteria for composition $\{CO_2(50\%),\ C_1(20\%),\ C_4(20\%),\ C_{10}(10\%)\}$ at $p = 1400$ psi and $p = 2300$ psi.

For all the computed critical tie-lines, we can find one with the minimal value of $F(L)$. Here L is found for each critical tie-line using (22). This tie-line is shown on Fig. 7 in light-green color. Using the point $\mathbf{z}(L)$ and the original composition $\mathbf{Z}$, we can decide if the composition belongs to the supercritical region or not. For this 'compositional check', we use the following procedure:

- Connect points $\mathbf{z}$ and $\mathbf{Z}$ with the longest tie-line $(\mathbf{x}, \mathbf{y})$ in the system (i.e. tie-line that belongs to vertices connected the lightest and heaviest components),
- For triangles $(\mathbf{z}, \mathbf{x}, \mathbf{y})$ and $(\mathbf{Z}, \mathbf{x}, \mathbf{y})$ (blue and red triangles on Fig. 7 respectively), calculate the lengths of the sides

$$l_1 = \|\mathbf{z} - \mathbf{x}\| + \|\mathbf{z} - \mathbf{y}\| \tag{23}$$
$$l_2 = \|\mathbf{Z} - \mathbf{x}\| + \|\mathbf{Z} - \mathbf{y}\| \tag{24}$$

– if $l_1 > l_2$, then the current composition $\mathbf{Z}$ is below the critical tie-line; otherwise, it is in a supercritical state.

For cases with significant pressure changes, the described approach is combined with a two-step procedure. The two sets of critical tie-line represent a critical surface for pressures $p^j < p^{j+1}$, where given $p \in [p^j, p^{j+1}]$. There are three possible cases for the state of composition $\mathbf{z}$ at pressure p:

1. for p^j, a supercritical state is identified.
2. for p^{j+1}, a subcritical state is identified.
3. for p^j, a subcritical state is identified, and for p^{j+1} a supercritical state is identified.

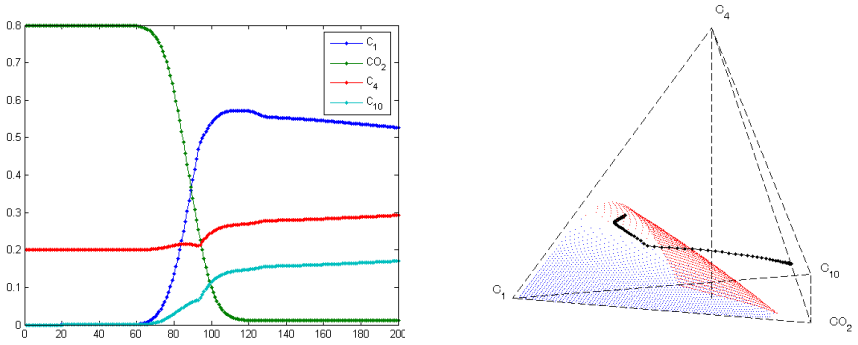
The first case guarantees that for $p > p^j$, the composition $\mathbf{z}$ is still above critical tie-line. The second case guarantees that for $p < p^{j+1}$, the composition $\mathbf{z}$ is below the critical tie-line. Only the third case requires additional criteria for supercritical state identification, where linear interpolation using the critical tie-line is employed.

The two parameterizations, namely, CSAT and SSC, are combined to provide a robust and computationally efficient treatment of phase behavior computations in general purpose compositional simulations. If a composition, in the pressure interval of interest, is in the region of tie-line extensions, CSAT identifies the phase-state and provides the phase compositions. If a composition is identified by SSC as supercritical, it is treated as in standard compositional simulation. Compared with the standard compositional simulation methodology, this compositional space parameterization framework leads to significant computational gains.

6. Combining CSAT with SSC: Results

The SSC method was implemented in the GPRS simulator. The following examples demonstrate the effectiveness of the SSC scheme as well as the effectiveness of combining it with CSAT. The first set uses four-component examples that were generated using the system $\{C_1,\ CO_2,\ C_4,\ C_{10}\}$. The second set involves five-component problems based on the system $\{C_1,\ CO_2,\ C_4,\ C_7,\ C_{10}\}$. All the examples are for 1D gas injection problems with different compositions and grid resolution.

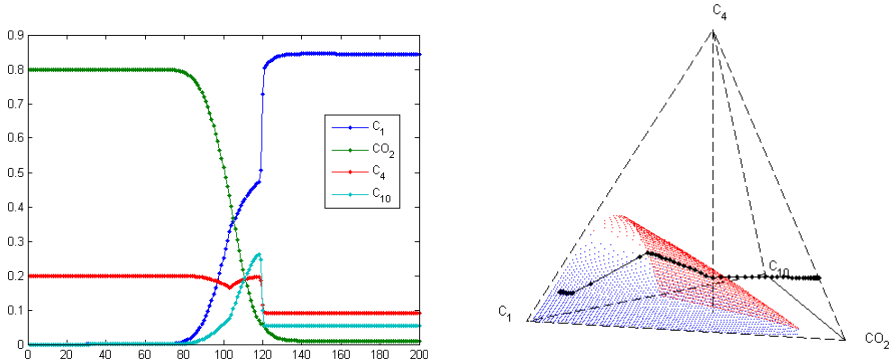
– Case 1: injection of gas $\{CO_2\ (80\%), C_4\ (20\%)\}$ into oil made up of $\{C_1\ (50\%),\ CO_2\ (1\%),\ C_4\ (25\%),\ C_{10}\ (14\%)\}$. The composition solution and projection of the solution on the phase diagram at reservoir pressure are presented in Fig. 8.



(a) **(b)**

Figure 8. Solution of Case 1 in standard (dimensional) and compositional space.

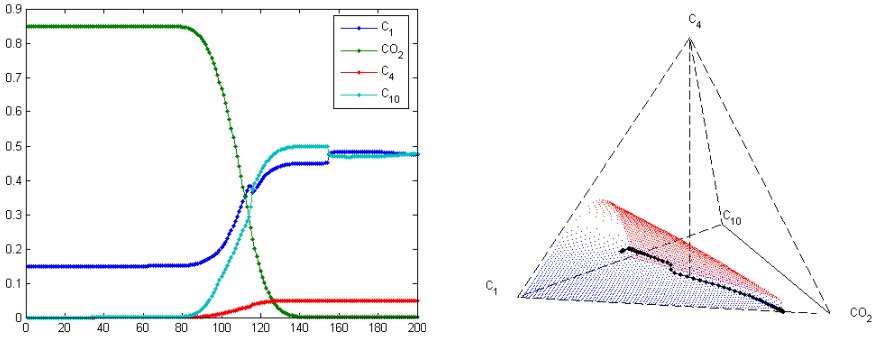
– Case 2: injection of gas $\{CO_2\ (80\%), C_4\ (20\%)\}$ into oil made up of $\{C_1\ (85\%),\ CO_2\ (1\%),\ C_4\ (9\%),\ C_{10}\ (5\%)\}$. The composition solution and projection of the solution on the phase diagram at reservoir pressure are presented in Fig. 9.



(a) **(b)**

Figure 9. Solution of Case 2 in standard (dimensional) and compositional space.

– Case 3: injection of gas $\{C_1\ (15\%), CO_2\ (85\%)\}$ into oil made up of $\{C_1\ (45\%),\ C_4\ (5\%),\ C_{10}\ (50\%)\}$. The composition solution and projection of the solution on the phase diagram at reservoir pressure are presented in Fig. 10.

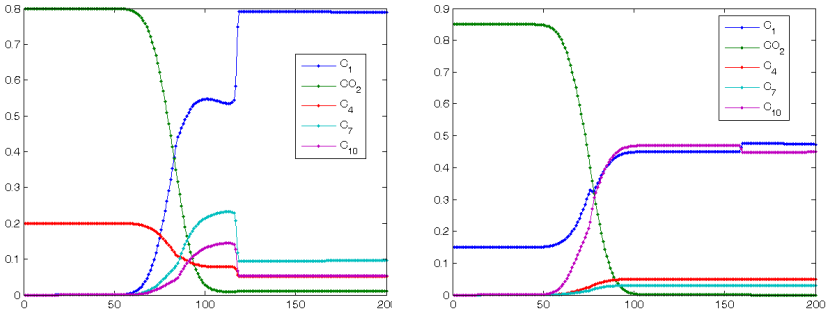


(a) **(b)**

Figure 10. Solution of Case 3 in standard (dimensional) and compositional space.

– Case 4: Analog of Case 2, but for a five-component system. Injection of gas $\{CO_2\ (80\%), C_4\ (20\%)\}$ into oil made up of $\{C_1\ (80\%),\ CO_2\ (1\%),\ C_4\ (5\%),\ C_7\ (9\%),\ C_{10}\ (5\%)\}$. The composition solution is presented in Fig. 11,a.

– Case 5: Analog of Case 3 but for a five-component system. Injection of gas $\{C_1\ (15\%), CO_2\ (85\%)\}$ into oil made up of $\{C_1\ (45\%),\ C_4\ (5\%),\ C_7\ (3\%),\ C_{10}\ (47\%)\}$. The composition solution is presented in Fig. 11,b.

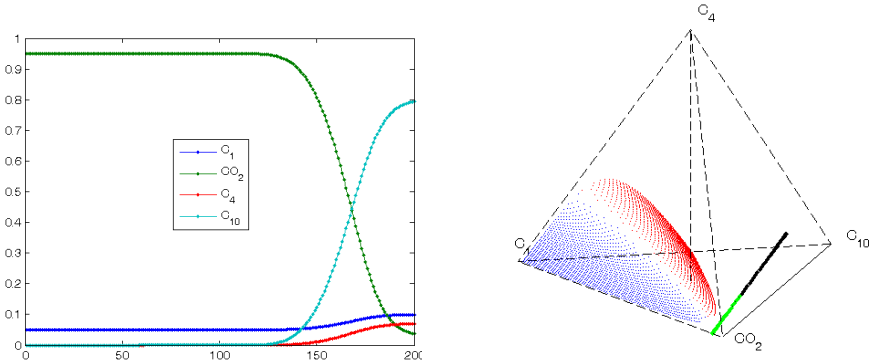


(a) **(b)**

Figure 11. Solution of Cases 4 and 5 in standard (dimensional) space.

– Case 6: This is a first-contact miscible injection of gas $\{C_1\ (5\%), CO_2\ (95\%)\}$ into oil made up of $\{C_1\ (10\%),\ CO_2\ (3\%),\ C_4\ (7\%),\ C_{10}$

(80%)}. The composition solution and projection of the solution on the phase diagram at reservoir pressure are presented on Fig. 12.



(a) **(b)**

Figure 12. Solution of Case 6 in standard (dimensional) and compositional space.

All the simulation are performed using GPRS in three different modes:

- Original - standard compositional model
- SSC - standard compositional model with SSC preconditioning
- SSC+CSAT - standard compositional model with SSC and CSAT preconditioning

The results of these calculations are presented in Table II. The stability iteration count includes phase stability tests, flash calculations, and surface-condition flashes (both SSI and Newton). CPU and EOS columns show total CPU time for simulation and time spent for EOS calculations respectively. CSAT field show number of checks and number of tie-lines parameterized.

Analysis of the results indicates that in most cases, the combination of SSC+CSAT gives the best results in terms of computational performance. Notice that the EOS time for all cases includes the time for tie-line parametrization needed by CSAT. This fact explains why EOS time for the cases with SSC+CSAT sometimes can be longer than the SSC time.

Further analysis indicates that CSAT performance improves when more tie-lines are used in the solution (e.g., Case 2). Moreover, as the

Table II. Comparison between standard, SSC, and SSC+CSAT simulation methods

Case	Type	Stab. it., 10^3	CPU, sec	EOS, sec	CSAT,10^3 (num)
Case 1	original	7917 + 1068	87.9	36.5	
	SSC	384 + 41	46.2	5.4	
	SSC+CSAT	232 + 33	40.9	9.8	5265 (7)
Case 2	original	13971 + 1882	157.0	62.7	
	SSC	1148 + 81	82.5	9.0	
	SSC+CSAT	642 + 69	80.7	13.3	6574 (3)
Case 3	original	17222 + 2971	154.7	86.0	
	SSC	7056 + 1620	106.0	48.1	
	SSC+CSAT	573 + 87	65.8	11.6	614634 (15)
Case 4	original	7641 + 1089	120.6	44.4	
	SSC	588 + 72	89.2	8.4	
	SSC+CSAT	488 + 66	90.5	17.1	5831 (3)
Case 5	original	16489 + 2788	165.9	104.4	
	SSC	5395 + 1229	101.8	53.1	
	SSC+CSAT	217 + 47	57.3	10.3	485654 (14)

immiscible part of the solution becomes smaller (e.g., Case 3), CSAT performance suffers a bit. The same observation holds for the five-component problems (Case 4 and Case 5), which were constructed using the four-component systems as a base.

The table III presents the dependency of the SSC method on the number of critical tie-lines used to represent the critical tie-line surface. For selecting the critical tie-lines, we use the length limit given by

$$l = \sqrt{\sum_{i=1}^{n_c} (x_i^c - y_i^c)^2} < \varepsilon. \tag{25}$$

For two cases Case 2 and Case 4, we present results of SSC performance for different ε. These results include the number of Newton iterations for simulation.

The performance of the SSC method as a function of the number of tie-lines used to represent the critical surface is quite reasonable. This is because the table search for the closest critical tie-line used in the SSC algorithm requires a linear number of operations. Moreover, a study of the solution path on the phase diagram shows that the path

Table III. Sensitivity of the SSC method on the number of tie-lines

Case	Type	Newton it.	Stab. it., 10^3	CPU, sec	EOS, sec
Case 2	$\varepsilon < 0.12$	6345	981 + 79	86.7	16.2
	$\varepsilon < 0.10$	6360	1065 + 80	85.0	11.3
	$\varepsilon < 0.08$	6342	1148 + 81	82.5	9.0
Case 4	$\varepsilon < 0.12$	4322	294 + 61	110.5	38.2
	$\varepsilon < 0.10$	4322	294 + 61	97.2	23.9
	$\varepsilon < 0.08$	4844	588 + 72	89.2	8.4

Table IV. Performance of SSC method versus resolution for modifications of Case 2

Blocks	Type	Newton it.	Stab. it., 10^3	CPU, sec	EOS, sec	Ratio
100	original	3787	4342 + 550	50.0	19.1	38.1%
	SSC	3529	488 + 43	28.8	2.9	10.2%
200	original	6930	13971 + 1882	157.0	62.7	40.0%
	SSC	6342	1148 + 81	82.5	9.0	11.0%
500	original	15734	73277 + 10671	772.4	339.9	44.0%
	SSC	14477	3714 + 199	427.3	44.8	10.5%

for multi-contact miscible problems always intersects the critical tie-line surface at a very limited number of points. This also means that localization methods may be useful.

The table IV presents the performance of SSC for different grid resolutions. This test was performed using the Case 2 setting. As you can see for this case, SSC always shows better performance (about an order of magnitude) for EOS time compared with the standard compositional method. Notice also that ratio of EOS time to total CPU time appears to be (largely) independent of the number of grid blocks for the SSC method and is about 10% for this case.

The last table presents two different first-contact miscible cases. Both cases are based on Case 6 with different resolutions. CSAT for these calculations was also run with different tolerance values.

As you can see, the SSC cost is minor because EOS calculations in supercritical region are quite limited. Note that CSAT shows good performance in this case, because the stability test in the single-phase

Table V. First-contact miscible displacement calculations for modifications of Case 6

Case	Type	Stab. it., 10^3	CPU	EOS	CSAT,10^3 (num)
Case 6	standard	9441 + 1557	66.0	44.3	
200	SSC	5195 + 1031	56.8	34.3	
blocks	SSC+CSAT(10^{-3})	80 + 16	53.3	30.0	1362 (20)
	SSC+CSAT(10^{-2})	80 + 16	39.0	18.0	971 (8)
Case 6	standard	43283 + 7517	303.0	209.7	
500	SSC	26304 + 5192	271.9	174.9	
blocks	SSC+CSAT(10^{-3})	165 + 33	172.2	84.8	5894 (20)
	SSC+CSAT(10^{-2})	165 + 33	141.0	53.0	4555 (7)

part of the tie-line extension consumes a lot of time. For cases with looser CSAT tolerance, the number of tie-lines involved decreases, and that is reflected in better EOS time (less tie-lines checked in the table).

7. Conclusions

We presented a multi-component, multi-phase, reservoir flow simulation methodology based on the parametrization of the compositional space using tie-lines. CST can be used to replace all phase behavior calculations (i.e., phase stability and flash calculations). The adaptive tabulation scheme, CSAT, can be used most effectively to replace the phase stability test in conventional EOS compositional simulators. CST and CSAT were implemented in a General Purpose Research Simulator (GPRS). Using a variety of challenging compositional gas-injection problems, we show that compared to standard approaches, CSAT leads to very large improvements (at least an order of magnitude) in the performance of phase behavior computations. We note that these tie-line based parametrization schemes can be incorporated into existing simulations relatively easily.

We then presented a parameterization of the critical tie-line surface. This parameterization makes it possible to determine whether a composition is supercritical or subcritical. The SSC parameterization complements the tie-line based CSAT strategy. This combination allows for robust and computationally efficient general purpose compositional simulations.

Acknowledgements

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