Compositional Space Parametrization: Multi-Contact Miscible Displacements and Extension to Multi-Phase

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Summary

In this work we generalize the Compositional Space Parametrization (CSP) approach, which was originally developed for two-phase compositional problems. This parametrization improves the accuracy of the phase behavior representation as well as the efficiency of various types of computation for compositional flow. One application of this approach is to speed up standard multi-component phase behavior computations. For general purpose compositional simulation, Compositional Space Adaptive Tabulation (CSAT) can be used to avoid most of the redundant Equation of State calculations. A Supercritical State Criteria algorithm, which is based on adaptive tabulation of the critical tie-simplex, is used to handle the super-critical region. Results of several challenging tests of practical interest indicate that the CSAT strategy is quite robust, and that it leads to an order of magnitude gain in computational efficiency. This strategy is valid for systems with any number of phases and components. Another application area for our CSP framework is to speed up standard thermodynamic computations for complex mixtures. For such systems, the methodology is generalized in terms of a multi-phase tie-simplex description, where one finds the closest tie-simplex and uses it as an initial guess for the computations. For better tie-simplex estimation, interpolation based on triangulation is used. For cases with wide variation in pressure and temperature, linear interpolation of the tie-simplex for these variables is adequate. The methodology is demonstrated using several challenging examples.

Introduction

Enhanced Oil Recovery (EOR) processes usually involve the injection of fluids in the reservoir to displace the resident, or remaining, oil. Multi-contact miscible gas injection displacements, for example, rely on the mass transfer between the injected and resident fluids to improve the local displacement efficiency. These reservoir displacement processes are usually modeled using the assumption of instantaneous thermodynamic equilibrium. Using a multi-component description of the fluid system (resident and injected), an Equation of State (EoS) is used to describe the complex phase behavior as a function of composition, temperature, and pressure. To model the complex nonlinear flow associated with EOR processes, numerical reservoir simulators solve the component mass conservation equations, the energy balance if necessary, thermodynamic equilibrium relations, and constraint relations, for the given discrete representation of the reservoir.

General-purpose reservoir simulators in wide use employ an EoS, or K-value tables, to perform the phase equilibrium calculations Coats (1980) - Aziz and Wong (1988). In compositional flow simulation, given the temperature, pressure, and overall composition in a gridblock at a particular time, phase behavior computations are used to (1) determine the phase state and (2) the phase compositions at equilibrium. The computational cost associated with these phase behavior calculations increases with the number of components used to represent the fluid system. Motivated by the need for more accurate performance predictions, the level of detail of reservoir characterization models has continued to grow. While black-oil simulation efficiency has kept up with the growth in reservoir model sizes, this is not the case for practical large-scale compositional simulation. In addition to dealing with highly detailed heterogeneous reservoir models, much of the difficulty is due to the complex nonlinear interactions associated with the transport of large numbers of components, which partition across multiple flowing fluid phases, as a function of space and time.

There are several efforts related to the work presented here. For example Wang et al. (1997) described a compositional reservoir simulator based on an IMPEC (IMplicit Pressure, Explicit Compositions) formulation. They used a *negative flash* (Li and Nghiem (1982), Whitson and Michelsen (1989)) procedure to perform both phase-state identification and flash. This method is equivalent to finding a tie-line (and its extension) and checking where the composition lies. A good initial guess is required for the method to be computationally efficient. Rasmussen et al. Rasmussen et al. (2006) presented a method to speed up the flash calculations and the phase stability test for compositional mixtures in pipe flow. They proposed criteria for avoiding the phase stability test for single-phase fluids, which is very efficient for transient simulation where the compositions change slowly.

In Voskov and Tchelepi (2007), we presented a tie-line based Compositional Space Parametrization (CSP) framework for immiscible compositional simulation. One can show that for a given pressure and temperature, the tie-line based representation can be interpreted as a coordinate transformation between standard compositional space and tie-line space. In practice, however, a discrete representation of the tie-line space is employed. The most effective use of this CSP framework in general-purpose compositional simulation is to build and adaptively update a *tie-line table*, where the parameters and phase compositions associated with a particular tie-line are obtained from the EoS. This Compositional Space Adaptive Tabulation (CSAT) strategy leads to significant gains in computational efficiency compared with standard EoS based compositional simulation Voskov and Tchelepi (2007).

Since by definition, one cannot define a tie line in the super-critical region (for fixed pressure and temperature, the zero length tie-line is the critical tie-line), direct parametrization of compositions in the super-critical region is not possible. This difficulty is overcome by parametrization of the surface of critical tie-lines. Using this surface, one can determine the phase state of a given composition (i.e if the composition lies in the region of tie-line extensions, or is super-critical). This strategy for identifying a composition as super-critical is referred to as the Super-critical State Criteria (SSC) (Voskov and Tchelepi (2008)). If a composition lies in the region of tie-line extensions, the standard CSAT scheme, in which a tie-line table is constructed adaptively (Voskov and Tchelepi (2007)), can be used to determine the phase-state and the phase compositions.

Here, we extend the work described in Voskov and Tchelepi (2007) and that of Voskov and Tchelepi (2008) in two important ways. First, we show that the parametrization of the critical tie-lines can be performed adaptively. Here, two tables are constructed and updated in the course of a compositional simulation: a *tie-line table*, and a *critical tie-line table*. This fully adaptive tie-line based parametrization framework, which we call CSAT (Compositional Space Adaptive Tabulation), is used to speed up EoS based simulation of multi-contact miscible displacement processes. This CSAT approach was implemented in a general-purpose compositional research simulator. We use several challenging compositional prob-

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lems to demonstrate the efficiency of the methodology. Second, we describe the extension of the Compositional Space Parametrization (CSP) framework for multi-component systems, in which three (or more) phases may be present at equilibrium.

Adaptive Tie-line Tabulation Modification

We employ a tie-line based parametrization. For the compositional space of interest, an appropriate EoS can be used to delineate the two-phase envelope and compute the tie-lines Voskov (2002), Voskov et al. (2001). For every point below the critical tie-line in the standard compositional space at fixed pressure and temperature, there exists a unique point in tie-line space. As the result, a continuous description in the tie-line space is possible. Here a discrete representation of the tie-line space is used. An (n_c-2)-dimensional γ-parameter is used to identify a particular tie-line. Any combination of fractions can be used as γ. For example, in Voskov et al. (2001) the γ-parameter is defined as the center point of a tie-line, $\gamma_i = 0.5(x_i + y_i)$. The only requirement is that each tie-line, including its extension, be identified with a unique and constant γ. Using this parameter, the equilibrium phase compositions associated with the specific tie-line are tabulated (e.g., fractions $x_i(\gamma)$ and $y_i(\gamma)$), and that provides a complete description of the phase behavior for any composition along the tie-line, or its extension.

One can also use an approximate representation of the tie-line space using polynomials Voskov et al. (2001). A more general approach is to pre-compute the tie-line space at discrete points. The compositional space can be covered by a mesh (e.g., Delaunay triangulation). Then tie-line interpolation is performed using the mesh where and when necessary (Voskov and Tchelepi (2007)). Complete and high-resolution discretization of the entire compositional space can be very expensive and is not necessary. This is because multi-component gas-injection reservoir displacements usually operate in a limited part of the compositional space, such that only a small subset of the tie-line space is involved in the solution path.

In the tie-line based parametrization approach, for the particular compositional displacement problem of interest, we choose a pressure range and a discretization interval. A *tie-line table* is constructed, where for a particular composition the tie-lines (i.e., equilibrium phase compositions) corresponding to each discrete pressure value are computed and stored. A negative flash procedure is used to parameterize the tie-lines as a function of pressure.

The negative flash was first presented by Li and Nghiem (1982) and then fully developed by Whitson and Michelsen (1989). This approach simple remove the limitations for mole fraction in the liquid and vapor phase (L and V respectively) be in $[0,1]$ interval in the flash computation procedure. The converged solution of such flash computation procedure in single phase region introduce parameters that define an extension of tie-line that intersect a given composition. Inside of the interval $[0,1]$ negative flash results are equivalent to normal flash. Whitson and Michelsen (1989) present an important limitation for the interval of definition for mole fraction. The CSAT approach can be seen as an efficient computation of initial guess for negative flash procedure.

For the tie-line parametrization we start from the lowest pressure in the range of interest, for which an initial guess is obtained from the Wilson correlation

$$K_i = e^{5.373(1+\omega_i)(1-T_{ci}/T)}\, p_{ci}/p. \qquad \ldots\ldots\ldots\ldots\ldots (1)$$

For subsequent (higher) pressures, the converged K_i values from the flash solution for the previous pressure serve as an initial guess to find and parameterize the next tie-line.

During flow simulation, whenever a phase stability test, or flash, is required, we check if the composition belongs to a tie-line in the table. To check the composition, we use the following equations

$$L = \frac{z_j - y_j}{x_j - y_j}, \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

$$\sum_{i=1}^{n_c} \left(x_i L + y_i(1-L) - z_i\right)^2 < \varepsilon. \qquad \ldots\ldots\ldots\ldots\ldots (3)$$

Here component j can be arbitrarily chosen. The values for x_i and y_i is computed at each tie-line set for a given pressure using linear interpolation. These expressions are inexpensive and add negligible overhead. If one of the stored tie-lines satisfies these equations for the composition of interest, the value of L is used for the flash results. If the composition does not lie on any of the stored tie-lines, a new tie-line is computed and added to the table.

A tolerance value is used in the tie-line intersection criterion (3), which can be interpreted as a cylinder of radius ε centered around the tie-line. If the composition is close to the two-phase boundary, there is no guarantee that the composition will be in the same state as the compositions of the supporting tie-line (see Fig. 1). This misidentification close to the two-phase boundary can lead to oscillatory behavior in the global Newton iterations, where the transport equations are solved. In order to avoid these difficulties, we perform additional negative flash calculations for compositions that are deemed close to the two-phase boundary. For a particular value of

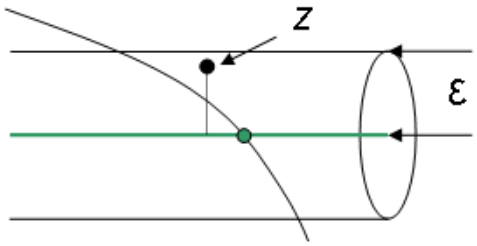


Fig. 1—Tie-line vicinity with supporting tie-line.

L from (2), we decide if composition $\mathbf{z}$ is close to the liquid or vapor boundary, $L > 0.5$ or $L < 0.5$, respectively. Then, we calculate the distance to the boundary

$$l = \sqrt{\textstyle\sum_i (z_i - w_i)^2}, \qquad \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

where w_i is the fraction of the phase obtained from the tie-line. If this distance is less than $N\varepsilon$ (where N is a small integer), we run an additional negative flash using an initial guess provided by the tie-line.

The results of CSAT method for compositional immiscible displacements are presented in Voskov and Tchelepi (2007). By immiscible, we mean that all the compositions along the solution are within the region of tie-line extensions throughout the displacement process. In this method we didn't use precision check based on negative flash for compositions close to the boundary of two-phase region. For some of the cases that leads to oscillation of a nonlinear iterations during simulation. It is become the big problem when the angle of two-phase boundary has very sharp angle with supporting tie-line that is usually the case for near-miscible displacement. In the next section, we describe a fully adaptive tie-line based treatment that is applicable for general-purpose simulation of near-miscible compositional displacements.

Adaptive Supercritical State Criteria

The adaptive tie-line tabulation approach described by Voskov and Tchelepi (2007) for compositions that lie within the region of tie-line extensions. Consequently, the method faces a fundamental difficulty in dealing with solution paths that cross the critical surface (see Fig. 2). Without additional guidance, the original tabulation scheme tries to find a tie-line, or its extension, even though the composition may belong to the super-critical region. In this case, convergence failure can be used to indicate a super-critical state. Then, standard EoS phase-stability computations can be used to identify the state more precisely. Such a strategy can be costly if supercritical compositions are encountered frequently during the course

of a high-resolution (large number of gridblocks) simulation. This can limit the utility of the parametrization approach in modeling multi-contact miscible displacement processes.

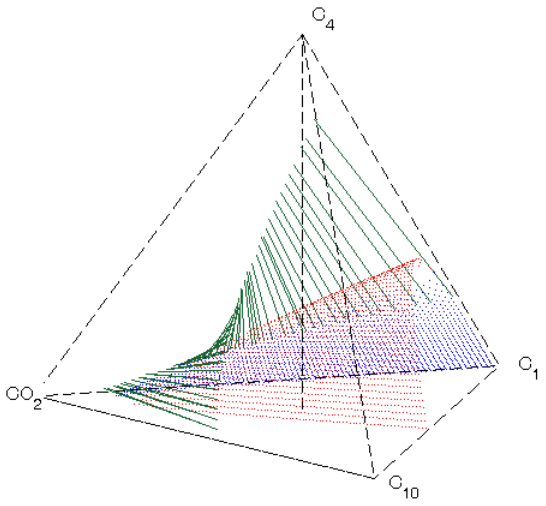


Fig. 2—Critical subsurface (green) for the system $\{CO_2, C_1, C_4, C_{10}\}$ at $p = 2350$ and $T = 160^oF$.

In order to overcome this problem, the critical surface can be parameterized and used to decide if a composition is sub- or super-critical. This Supercritical State Criteria (SSC) approach was described by Voskov and Tchelepi (2008). That method is based on precomputation of the tie-lines using pseudo-ternary slices of the compositional diagram (Voskov et al. (2001), Voskov (2002)) where the last computed tie-line in each pseudo-ternary slice is close to the critical one within a predefined tolerance. So the first step of the SSC approach (Voskov and Tchelepi (2008))is to collect all the critical tie-lines.

To determine if a composition is sub- or super-critical, we have to find if the composition in multi-dimensional space is above or below the critical tie-line surface (see Fig. 2). For all critical tie-lines we need to find the distance to the given composition and choose the closest tie-line. A simple geometrical check is used for this purposes. If the composition is sub-critical (i.e., within the region of tie-line extensions), the tie-line tabulation procedure (Voskov and Tchelepi (2007)) is used. If a composition is super-critical, standard correlations can be used to further identify the mixture state as vapor-like or liquid-like (see Gosset et al. (1986) for example).

Several issues are associated with this SSC approach. First, for mixtures with large numbers of components, it is not obvious how to delineate the critical tie-line surface accurately and efficiently. Another source of difficulty is interpolation of the critical tie-line surface as a function of pressure. The third source of difficulty is that further identification of the super-critical mixture state as vapor-like or liquid-like using standard correlations can lead to erroneous results. For example, Fig. 3 shows part of the solution route for a super-critical gas injection problem. The standard approach (Gosset et al. (1986)) leads to misidentification of the phase state as a super-critical liquid long before actually crossing the critical line.

Here, we propose an adaptive SSC strategy, that does not require the construction of the critical surface. The critical tie-lines are computed as needed and stored in a separate *critical tie-line table*. In a manner similar to the original tie-line tabulation approach (Voskov and Tchelepi (2007)), parametrization of the tie-lines as a function of pressure is performed by starting with the lowest pressure in the range of interest, and proceeding to the next pressure value. Failure of the parametrization procedure for a composition at pressure p^j (i.e., no tie-line is found) indicates that the Minimal Critical Pressure (MCP) of the mixture lies between p^{j-1} and p^j. Here MCP is defined as the minimal pressure for which the composition is intersected by a critical tie-line at fixed temperature. Then, a search scheme (e.g., bisection) can be used to locate the critical tie-line, which we take as the tie-line limited by the following minimal and maximal lengths

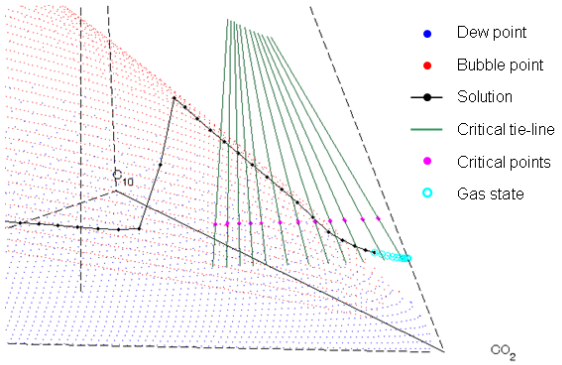


Fig. 3—Supercritical $\{CO_2, C_4\}$ gas injection (part of the Eclipse solution) with corresponding critical tie-lines and critical loci. Part of the solution interpreted as a gas marked (○).

$$\varepsilon_1 < \sqrt{\sum_i (x_i - y_i)^2} < \varepsilon_2. \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

The critical tie-line and the corresponding MCP are added to the *critical tie-line table*. With this adaptive MCP based approach, the same procedure is used to find and parameterize both the critical and immiscible (within the region of tie-line extensions) tie-lines. So, by adaptively updating a tie-line table and a critical tie-line table, we can handle sub- and super-critical compositions in the course of a simulation. Fig. 4 shows the solution of a four-component miscible gas injection problem in compositional space with parameterized critical tie-lines and corresponding MCPs. The phase state for any composition can be checked using the same criteria (2)-(3) for critical tie-lines.

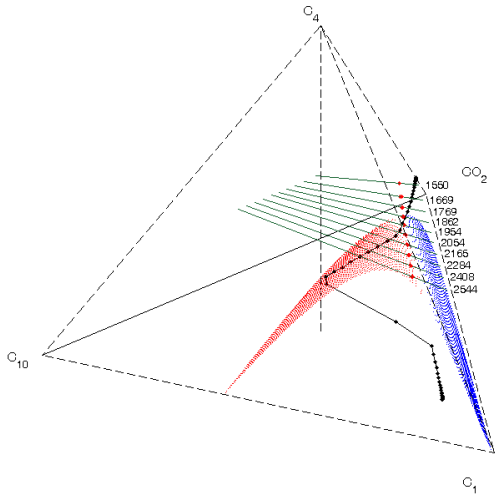


Fig. 4—Supercritical gas injection with corresponding critical tie-lines and MCP values. The solution path is shown in black dots. The critical tie-lines, along with the corresponding MCP values, are shown in green.

Notice that no pressure interpolation is necessary for a critical tie-line, because it is defined for a fixed value of pressure, namely, the MCP. If one of the critical tie-lines intersects the composition, and

the pressure in the gridblock is larger than the MCP, the composition state is identified as super-critical. Further state identification (as gas-like or liquid-like) is then based on the L obtained from (2) for a critical tie-line.

For state identification, we use the assumption that the state for the composition at a pressure larger than MCP (that means composition is in in critical conditions) is the same as the state at the MCP. This assumption is a reasonable approximation compared with the standard criteria (e.g. Gosset et al. (1986)) commonly used for super-critical state identification in compositional reservoir simulators. The use of this assumption can simplify and speed up the critical phase identification, since at MCP the composition is intersected by a critical tie-line, and the position on this tie-line defines the state of the composition.

If a critical tie-line intersects the composition in the gridblock but the pressure is less than the MCP, then the critical tie-line table look-up procedure is terminated. This is because the composition belongs to the part of the compositional space that is covered by the regular (i.e.,sub-critical) tie-line table. We retain the name Compositional Space Adaptive Tabulation (CSAT) in this paper to refer to the adaptive framework of parameterizing the entire compositional space, including the super-critical region.

The critical tie-line parametrization for a given temperature is also thermodynamically unique. Otherwise a given composition would have more than one critical point for the same temperature. As discussed in Voskov and Tchelepi (2007), when the pressure associated with the composition of interest is close to the MCP, the errors associated with tie-line table interpolation are sensitive to the pressure interval used. To avoid these interpolation difficulties, refinement of the pressure interval close to the MCP is used.

CSAT for Multi-Contact Miscible Simulation

Examples of the original sub-critical CSAT technique are described in Voskov and Tchelepi (2007). The combination of sub-critical CSAT with pre-computed SSC (Supercritical State Criteria) was tested for several challenging multi-contact miscible gas injection problems (Voskov and Tchelepi (2008)). In those examples, the number of components was small (four and five components).

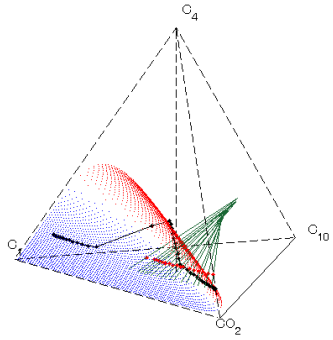
Here we demonstrate the complete adaptive parametrization for multi-contact miscible gas injection processes involving large numbers of components. All computations were performed using a General Purpose Research Simulator (GPRS) (Cao (2002)).

Critical Tie-line Distribution. The test cases are built based on the four-component system $\{CO_2, C_1, C_4, C_{10}\}$. A gas mixture $\{CO_2$ $(90\%), C_4$ $(10\%)\}$ is injected into oil composed of $\{CO_2(1\%), C_1(20\%),$ $C_4(29\%), C_{10}(50\%)\}$. At this condition the displacement process is multi-contact miscible. We choose the four component system in order to present the CSAT results on a compositional diagram. Two homogeneous cases are presented:

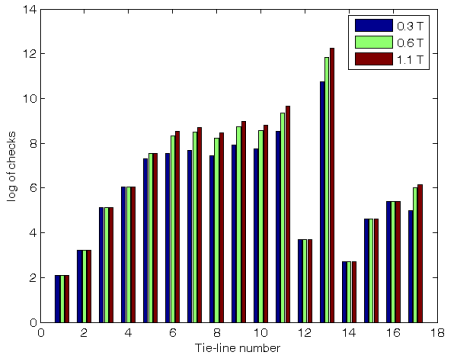
- A one dimensional (100 cells) problem with injection and production wells in the first and last grid blocks, respectively
- A three dimensional ($10 \times 10 \times 3$) problem with injection and production wells at the corners

For both tests, injection and production wells operate at Bottom Hole Pressure control of $p = 2600$ and $p = 1500$ psi, respectively. The interval used for CSAT parametrization is between $p = 1000$ and $p = 2700$ psi in order to safeguard the MCP computation for critical tie-lines.

Fig. 5(a) shows the solution of the one-dimensional problem in compositional space. For this case, CSAT collects 17 critical tie-lines during the simulation. All of these tie-lines were used for SSC checks during the simulation. Fig. 5(b) shows the number of checks for each tie-line at different times. Here T is gas breakthrough time for the model. In this case all the critical tie-lines are calculated in the beginning of the displacement process, and only half of them are used for supercritical identification throughout the simulation. The rest is computed and used only on the stage when critical part of the solution is developed.



(a)



(b)

Fig. 5—(a) 1D multi-contact miscible gas injection solution in compositional space, blue and red are dew and bubble points respectively for $p = 2000$ psi; (b) is a diagram for critical tie-line checks at three different times.

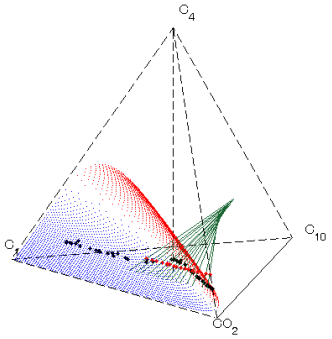
The next test is a 3D modification of the case just presented. The number of critical tie-lines collected by adaptive SSC is 15. The position of critical tie-lines (see Fig. 6(a)) is almost the same. For this simulation, the a smaller number of critical tie-lines (4) was used during the early stages of the displacement(see Fig. 6(b)). That happens because the 3D solution is more dispersive. But still the total number of tie-lines used for adaptive SSC is small.

The next simulation set is built from the fluid description of the SPE 3 problem. The original SPE 3 case is an immiscible depletion problem, where the initial composition is very close to the dew-point. The oil is composed of nine components $\{CO_2$ (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} $(40.3\%)\}$. We added a well that injects a mixture of gases at multi-contact miscible conditions ($\{CO_2$ $(90\%), C_3$ $(10\%)\}$. Two homogeneous configurations are used:

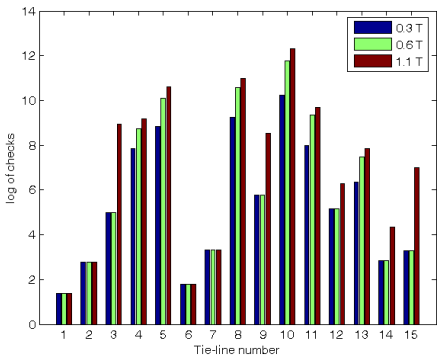
- A one dimensional (100 cells) problem with injection and production wells in the first and last grid blocks, respectively
- A three dimensional ($10 \times 10 \times 5$) problem with injection and production wells at opposite corners

For both tests, injection and production wells operate with Bottom Hole Pressure control at $p = 3000$ and $p = 1000$ psi, respectively. The CSAT interval was chosen between $p = 500$ and $p = 3200$ psi in order to safeguard the MCP computation for all the critical tie-lines.

In Fig. 7(a) you can see a distribution of critical tie-line checks for the one-dimensional gas injection problem at different times. Here several critical tie-lines (5-th, 9-th and 10-th) were used only once for SSC checks. Fig. 7(b) shows a diagram of the tie-line distribution for the 3D model at different times. Again you can

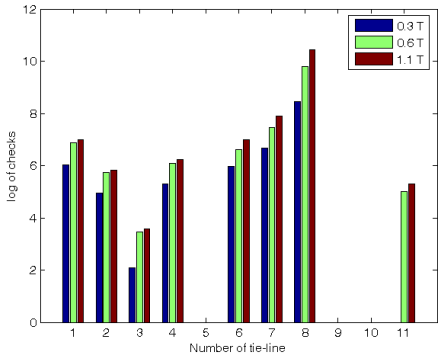


(a)

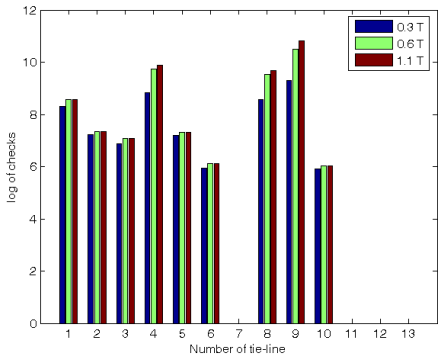


(b)

Fig. 6—(a) 3D multi-contact miscible gas injection solution in compositional space, blue and red are dew and bubble points respectively for $p = 2000$ psi; (b) is a diagram for critical tie-line checks at different times of simulation.



(a)



(b)

Fig. 7—SPE 3 diagram for critical tie-line checks for 1D (a) and 3D (b) multi-contact miscible gas injection cases.

see that only a few additional tie-lines are added, but the overall behavior is quite similar to the 1D displacement problem.

These examples demonstrate an important characteristic: just as in the case of similar to sub-critical (immiscible) tie-line distribution, critical tie-lines needed for adaptive SSC check are limited in number and concentrated in a small portion of the compositional space.

Results of Multi-contact Miscible CSAT. The next simulation set is again obtained using a modification of the SPE 3 problem (Kenyon and Behie (1983)). We added a miscible-gas injection well. The second set uses the SPE 5 Water Alternating Gas (WAG) injection problem (Killough and Kossack (1987)). We changed the injection composition to make the problem more miscible. Finally, we present a case where gas is injected in a fractured reservoir. The geometrical description of this reservoir as well as the details of the discretization are presented by Gong et al. (2007).

All the simulations, except for the second run, are obtained using a fully implicit method. Standard EoS-based phase behavior computations are performed based on combination of SSI and Newton.

- Case 1: modification of the SPE 3 test case: injection of a miscible gas mixture composed of $\{CO_2\ (90\%), C_3\ (10\%)\}$ 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 $10 \times 10 \times 5$ gridblocks, is used. Gas is injected in one corner at 3000 psi. The production well is in the opposite corner operating at 1000 psi.
- Case 2: same as Case 1, but in AIM (Adaptive Implicit Method) mode, where 90% of the gridblocks are IMPSAT (IMPlicit SATurations, explicit compositions) Cao (2002) and 10% are fully implicit.
- Case 3: a modified version of the SPE 5 WAG injection problem: the reservoir model is made up of $7 \times 7 \times 3$ gridblocks. Gas is composed of $\{C_1\ (70\%), C_3\ (20\%), C_6\ (10\%)\}$. The oil composition is $\{C_1\ (50\%), C_3\ (3\%), C_6\ (7\%), C_{10}\ (20\%), C_{15}\ (15\%)\}$, $C_{20}\ (5\%)\}$. Water and gas are injected in one corner at 5000 psi. The production well is in the opposite corner operating at 3000 psi. The injected gas is multi-contact miscible with the resident oil for the pressure interval of interest.
- Case 4: gas injection into a 3D fractured reservoir. The model contains 5227 unstructured gridblocks, which describe both the matrix and 30 explicit fractures. The fracture to matrix permeability ratio is 10^7; the initial oil and injected gas are composed of $\{H_2S, C_1, C_{2-3}, C_{4-7}, C_{8-26}, C_{39}\}$ pseudo components. Gas injection is first-contact miscible for the pressure interval of interest, namely, 11,000 to 12,500 psi.
- Case 5: same as Case 4, but with the production well operating at constant bottom-hole pressure that is below the bubble point pressure. The gas injection process is multi-contact miscible for the pressure interval of interest (2400 - 12500 psi).

Table 2 shows the standard and CSAT simulation results for these five cases. The numerical results of these simulations using both CSAT and the standard approach are practically indistinguishable (up to 10 significant figures). For some of the cases, CSAT procedure was run with a smaller tolerance (fCSAT in the second column indicate smaller ε in (2)). The stability iteration column includes the cumulative number of iterations (in thousands) needed for phase stability tests, flash calculations, and surface-condition flashes (SSI

Table 2—Test results for near-miscible gas injection

N	Type	Stab. iter., 10^3	CPU	EoS	TL (crit)
1	original	5365 + 886	78.0	47.0	-
	CSAT	49 + 12	37.1	2.4	50 (12)
	fCSAT	49 + 12	43.0	4.9	160 (35)
2	original	8910 + 1458	116.2	79.2	-
	CSAT	61 + 14	37.2	3.1	42 (5)
	fCSAT	64 + 15	48.4	6.9	159 (37)
3	original	11363 + 1605	102.5	58.0	-
	CSAT	87 + 20	67.9	12.7	9 (7)
	fCSAT	88 + 20	53.6	1.6	24 (18)
4	original	8492 + 4064	204.3	81.1	-
	CSAT	225 + 81	125.5	1.6	3 (3)
5	original	212381 + 55165	2351.0	1504.1	-
	CSAT	272 + 97	658.3	18.6	5 (4)

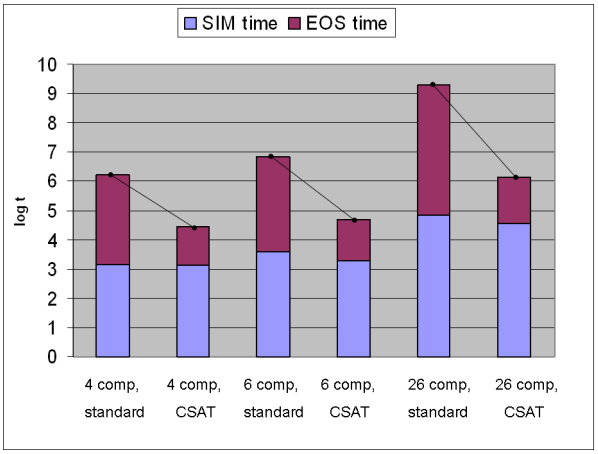


Fig. 8—EoS and simulation (Total - EoS) time for standard and CSAT simulation.

+ Newton). The next two columns show the total CPU time and the time spent on EoS calculations. The tie-line column lists the total number of tie-lines used in a simulation; the number of critical tie-lines is shown in parenthesis.

For the first three cases, CSAT was run with two different values for the tolerance. You can see that this parameter could be varied to obtain the best performance in terms of EoS computations. There are also several other parameters that can affect the performance and robustness of the CSAT method (e.g., criteria for switching from SSI to Newton in the negative flash). An optimal choice of these various parameters is beyond this paper and is likely to evolve as experience with the CSAT approach grows. This is similar to the various tolerances associated with the global Newton iterations in a general-purpose standard reservoir simulator. A detailed analysis of the table indicates that for most of the cases, CSAT with a reasonable parameter set improves the EoS calculation times by several folds. For the most challenging problem, Case 5 (multi-contact miscible gas injection with a large pressure range), the improvement in the EoS time is close to 100 times and total CPU improvement is more than 3 times.

Test case 4 was also run for different numbers of components. The fluid system was represented using 4, 6 and 26 components. All three models were run in standard and CSAT mode. Fig. 8 plots the log_{10} of the elapsed time for these simulations, which clearly shows that CSAT always improves EoS time by at least one order of magnitude for the simplest case and more than two orders of magnitude for the 26-component problem. In fact the EoS time for the CSAT simulation is a small fractions of the total time.

CSP for General Multi-Phase Systems

In this section, we extend the Compositional Space Parameterization (CSP) approach for any number of fluid phases. The CSP approach based on preprocessed (regularly or adaptively) tie-lines and criteria for tie-line to intersect composition (2)-(3). For multi-phase case this criteria can be extended. Tie-simplex $\mathbf{x}$ introduce multi-phase equilibrium region (e.g. tie-triangle for three-phase) and intersects the composition $\mathbf{z}$ if it satisfied

$$z_i - \sum_{j=1}^{n_p} \nu_j x_{i,j} = 0, \quad i = 1,\ldots,n_c-1, \quad \ldots\ldots\ldots \quad (6)$$

$$\sum_{j=1}^{n_p} \nu_j - 1 = 0. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

Notice that we have n_c-1 independent z_i.

Consider a subspace J of $\{1,\ldots,n_c-1\}$ with dimension n_p-1. The vector ν is the solution of

$$\begin{bmatrix} x_J \\ e \end{bmatrix} \nu = \begin{bmatrix} z_J \\ 1 \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (8)$$

where e is the unit vector $e = [\ 1, \quad \ldots, \quad 1\ ]$. We define the matrix $\begin{bmatrix} x_J \\ e \end{bmatrix} = C$ and write the solution of (8) as

$$\nu = C^{-1} \begin{bmatrix} z_J \\ 1 \end{bmatrix} = \alpha z_J + \beta. \quad \ldots\ldots\ldots\ldots\ldots \quad (9)$$

Here α is a matrix $[n_p \times (n_p-1)]$, β is a vector of size $[n_p]$.

Let $I = \{1,\ldots,n_c-1\}/J$. Then, we can write the following expression

$$z_I = x_I \nu = x_I C^{-1} \begin{bmatrix} z_J \\ 1 \end{bmatrix} = D \begin{bmatrix} z_J \\ 1 \end{bmatrix} = A z_J + b, \quad (10)$$

where the matrix D is defined as $D = [\ A \quad b\ ]$. Here A is a matrix $[(n_c-n_p)\times(n_p-1)]$, and b is a vector $[n_c-n_p]$. Notice that the matrix D is based on a nonlinear combination of the phase mole fractions, $x_{i,j}$, and that it can be uniquely defined based on thermodynamic equilibrium considerations. That means, the matrix D can be defined uniquely as a function of the thermodynamic vector γ whose dimension is $[n_c-n_p]$.

Here, we present preliminary results for the parametrization of a multi-phase multi-component system based on constant K-values that describe up to three phases. This assumption is used only to generate a simple example and not corresponds to any limitation of the multi-phase CSP method. For such a system, the general problem of phase equilibrium computation can be reduced to n_p-1 Rachford-Rice type equations and one constraint, namely,

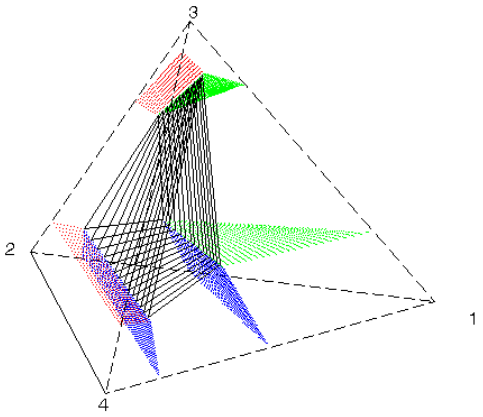
$$\sum_{i=1}^{n_c} \left(\frac{z_i(K_{i,j}-1)}{1+\sum_{k=1}^{n_p-1} \nu_{k+1}(K_{i,k}-1)} \right) = 0, \quad \ldots\ldots\ldots \quad (11)$$

$$\sum_{j=1}^{n_p} \nu_j - 1 = 0. \quad \ldots\ldots\ldots\ldots \quad (12)$$

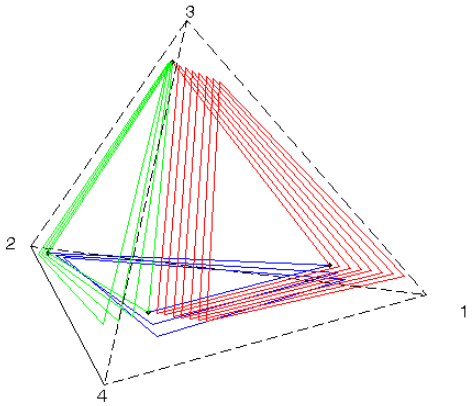
To solve this system of equations, we use the Newton method. The initial guess is taken as the barycenter coordinates $\nu_j = 1/n_p$. We will refer to this method as the standard solution.

The starting point of the parameterization is the construction of a discrete number of *tie-triangles* in the compositional space. We use an approach similar to that used for complete pre-calculation of the tie-lines Voskov et al. (2001). An example is shown in

Fig. 9. Here you can see parameterized tie-triangles and tie-lines for three-phase system and tie-tetrahedron and tie-triangles for four-component system.



(a)



(b)

Fig. 9—Tie-simplex set for highest and lower dimension for three-phase (a) and four-phase (b) systems.

For any given composition, **z**, in three-phase system we first find the closest tie-triangle using the equation

$$\min_t(z_I - A_t z_J + b_t), \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (13)$$

where A_t and b_t correspond to parameterized tie-triangles. Once the closest tie-triangle is found, it serves as an initial guess for the solution of the system (11). Based on this solution, we can determine if the composition belongs to the two-phase region, and if it does, we perform a two-phase flash. We parameterize the tie-lines associated with each tie-triangle. In Fig. 9, thick colored points correspond to the tie-line end points for each of the two-phase regions. These tie-lines also can be used as an initial guess for the two-phase flash.

We test several systems with different numbers of components. For randomly generated compositions, the standard solution of (11) and the CSP based solution were obtained. Fig. 10 shows the average number of Newton iterations for $n = 10^5$ randomly generated compositions. CSP based solutions were obtained for different tie-triangle densities (here the density parameter is the distance between tie-triangles). We also use two different CSP preconditioning methods based on the closest tie-triangle and on tie-triangles interpolation.

Our examples in this section are limited to constant K-values.

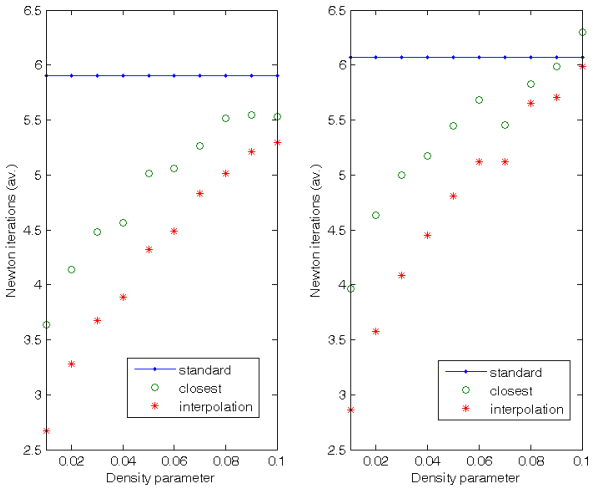


Fig. 10—Average number of Newton iteration for standard and CSP based preconditioning vs density of tie-triangles for 5 and 6 component constant K-values cases.

However this is not a limitation of the method and any type of phase equilibrium computation that uniquely defined tie-triangles in the three-dimensional phase subspace can be used instead. For of pressure and temperature variations, simple linear interpolation of tie-triangles can be used.

Conclusions

We presented an adaptive tie-line based compositional space parameterization framework for numerical simulation of multi-phase multi-component reservoir displacement processes. A fully adaptive strategy is used to parameterize a composition, at a particular pressure and temperature, whether it belongs to the sub- or super-critical region. In this CSAT (Compositional Space Adaptive Tabulation) approach, two tables are constructed and adaptively updated in the course of a simulation run.

The first is a *tie-line table*, where the tie-lines are parameterized as a function of pressure (and temperature) and stored. At any stage in the simulation, if the composition of interest is not in the tie-line table (either on one of the tie-lines or can be interpolated using existing tie-lines), then an appropriate EoS is used to locate and parameterize a new tie-line, which is then added to the table. The second table stores the *critical tie-lines*. The critical tie-lines are collected and stored in the course of tie-line parameterization as a function of pressure. Namely, if the MCP is encountered within a pressure interval, a critical tie-line is indicated, which is then pinpointed and stored. The critical tie-line table, which is adaptively updated, is used to identify the phase-state of a mixture at a given pressure and temperature. If the composition is sub-critical, then the (regular) tie-line table is used to look up the equilibrium data for the composition. The table is updated as needed when a composition cannot be resolved using the existing tie-lines.

The CSAT approach is demonstrated using several challenging compositional reservoir simulation problems. The examples include multi-component model problems as well as practical field problems. Near-miscible behaviors are simulated and compared with reference (i.e., standard EoS) computations. Overall, using CSAT for the phase behavior in general-purpose simulation is about an order of magnitude faster than conventional EoS based computations.

Finally, we showed that the CSP methodology can be extended to systems where components partition among three, or more, fluid phases at equilibrium. The idea is demonstrated for three-phase systems with constant K-values. In these cases, *tie-triangles* represent the equilibrium compositions in the three-phase region. Pre-

computation of the tie-simplex space is used to represent the phase behavior as a function of pressure and temperature. However, an adaptive strategy, similar to that used for multi-component two-phase systems, can be used for displacement problems where three, or more, phases may be present.

Nomenclature

p	Pressure
T	Temperature
z_i	overall mole fractions of component i
x_i	oil mole fractions
y_i	gas mole fractions
L	liquid phase volumetric fraction
V	vapor phase volumetric fraction
$f_{i,V}$	fugacity of component i in vapor phase
$f_{i,L}$	fugacity of component i in liquid phase
A_i	parameters for tie-line representation
B_i	parameters for tie-line representation
γ	tie-line parameter
ε	tolerance for tabulation
ν_j	volumetric fraction for phase j
K_i	equilibrium constants for component i
p_{ci}	critical pressure for component i
T_{ci}	critical temperature for component i
ω_i	acentric factor for component i

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