COMPOSITIONAL SPACE PARAMETERIZATION METHODS
FOR THERMAL-COMPOSITIONAL SIMULATION

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Rustem Zaydullin
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I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(Hamdi A. Tchelepi)  Principal Adviser

I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(Denis Voskov)

I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(Anthony R. Kovscek)

Approved for the University Committee on Graduate Studies
Abstract

Compositional simulation is necessary for the modeling of complex Enhanced Oil Recovery processes (EOR), such as gas and steam injection. Accurate simulation of these EOR processes involves coupling the nonlinear conservation laws for multicomponent, multiphase flow and transport with the equations that describe the phase behavior of the mixture at thermodynamic equilibrium. Phase-behavior modeling requires extensive computations and consumes significant time. The computational cost associated with the phase-behavior calculations increases significantly for systems where three or more fluid phases coexist at equilibrium.

We present a family of methods for the computation of the thermodynamic phase-behavior associated with multicomponent, multiphase flow in porous media. These methods are based on concepts developed in the analytical theory of one-dimensional gas-injection processes. For two-phase compositional simulation, we present a Compositional Space Parameterization (CSP) framework, in which the thermodynamic phase-behavior is reformulated in the tie-simplex space as a function of composition, pressure, and phase fractions. This tie-simplex space is then used to specify the base nonlinear variables for fully-implicit compositional simulation. The tie-simplex space is discretized, and multilinear interpolation of the thermodynamic relations is employed. Thus, all the thermodynamic properties become piece-wise linear functions in the tie-simplex space. The computation of the phase behavior in the course of a compositional simulation then becomes an iteration-free procedure and does not require any Equation of State (EoS) computations (flash computations or phase-stability tests). We demonstrate that the proposed CSP method reduces the computational cost of the thermodynamic calculations significantly compared with standard EoS-based approaches. Moreover, the proposed framework is promising not only for
acceleration of phase-behavior computations, but more importantly as a new thermodynamically consistent approximation for general-purpose compositional simulation.

Next, for the general case of multiphase (three, and more phases) simulation, we study the importance of using EoS-based modeling for thermal reservoir simulation. Here, the EoS-based approach is compared with the industry standard K-values method. The analysis employs simple one-dimensional thermal displacements of heavy oil by a mixture of steam and solvent. This analysis shows that three-phase EoS-based computations may be necessary for accurate modeling of certain types of thermal EOR processes.

Finally, we develop an extension of the CSP framework for multicomponent, multiphase thermal-compositional simulation. In particular, we present a strategy for phase-state identification that can be used to bypass the need for full three-phase EoS computations. The method uses information from the parameterized extensions of the ‘key’ tie-simplexes and is based on the adaptive discretization of the extensions of these tie-simplexes. We demonstrate the efficiency and robustness of the developed bypass strategy for the simulation of flow and transport in thermal, three-phase compositional models of heterogeneous reservoirs.
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Chapter 1

Introduction

Compositional modeling of field-scale recovery processes continues to be a challenging reservoir simulation problem. Field-scale models tend to be geometrically complex, with highly detailed spatial distributions of the formation properties. Moreover, the number of components used to represent the fluid system can be large.

Compositional simulation involves solution of a coupled system of nonlinear conservation laws for multicomponent, multiphase systems. A nonlinear system of thermodynamic constraints is used to represent the instantaneous phase equilibrium of the mixture. An Equation of State (EoS) model is usually employed to describe the phase behavior (Aziz and Wong, 1989; Lake, 1989) of a multicomponent mixture. For a given temperature, pressure, and overall composition, EoS computations yield the phase state (stability test), and the composition of each phase (flash calculation). Since EoS computations must be performed for each computational cell and for each global Newton iteration, these computations can consume a significant fraction of the total computational time.

An important advance in the understanding of compositional displacements has been achieved during the development of the analytical theory of gas injection (Dindoruk et al., 1997; Orr et al., 1993; Orr, 2007). The theory applies for one-dimensional (1D) hyperbolic (fixed pressure and temperature) compositional displacement of oil by miscible gas injection. Using the Method of Characteristics (MOC), it has been shown that the displacement can be fully described by a few key tie-lines (Orr, 2007). The solution structure is controlled by the fractional-flow characteristics along the
paths of these key tie-lines and the eigenvalues for the non-tie-line part of the solution. Another key finding from gas-injection theory is a proof that miscible displacement can be achieved only if the solution path crosses a critical tie-line (a zero-length tie-line). These theoretical findings are used as building blocks in our compositional space parameterization framework.

We present methods for efficient simulation of displacement processes associated with different types of Enhanced Oil Recovery (EOR) methods, such as miscible gas injection, steam and steam-solvent flooding, and Steam-Assisted Gravity Drainage (Butler et al., 1981). We refer to the developed approaches as Compositional Space Parametrization (CSP) methods. The CSP-based methods discussed in this work are developed for isothermal and thermal compositional EOR simulations; moreover, we not only focus on conventional two-phase compositional simulation, but also on challenging three-phase problems.

The CSP method is integrated in Stanford’s Automatic Differentiation General-Purpose Research Simulator (ADGPRS) (Younis, 2011; Zhou, 2012; Voskov and Tchelepi, 2012). The simulator has been significantly restructured in order to be able to perform challenging simulations that involve EoS- and K-value based thermal simulation, including low-temperature CO$_2$ injection.

1.1 Compositional Space Parameterization (CSP) for Two-Phase Compositional Simulation

Isothermal compositional models are described by a set of nonlinear equations that include mass conservation equations (one per component) and thermodynamic equilibrium constraints. The phase-behavior of hydrocarbon mixtures is usually described using an Equation of State (EoS) model. The EoS-based phase-behavior computations can be split into two procedures: phase-stability testing (Michelsen, 82a) and flash computations (Michelsen, 82b). These computations need to be performed for each global Newton iteration.

An important aspect of any compositional model is the choice of the primary variables used to solve the governing equations. There are several choices for the primary variables; the various (nonlinear) formulations are usually identified according to the
specific variable-set used. The two most widely used formulations are: the Natural Variables (Coats, 1980a) and Molar variables (Acs et al., 1985; Chien et al., 1985). In general, the nonlinear performance of a particular formulation depends on the details of the problem being solved (Farkas, 1998; Voskov and Tchelepi, 2012).

Since the phase-behavior computations can be quite time consuming, different methods to improve the efficiency of compositional flow simulation are discussed in the literature. In cases where the phase-behavior is a weak function of composition, a model based on constant K-values can be used (Bolling, 1987). Despite its great efficiency, this method does not allow for accurate modeling of complex compositional processes, such as multi-contact miscible displacements. This is because the standard K-values method relies on the assumption that the K-values are independent of composition. As has been shown in the analytical theory of miscible gas injection, part of the solution path lies in a region where strong compositional effects are present; therefore, the standard K-values approach results in substantial errors in the phase-behavior representation for these displacements.

When the natural-variables formulation is used, phase-stability testing makes up the bulk of the EoS computations in a typical compositional simulation. Several research efforts related to the use of reduced variables for phase-stability computations (Michelsen, 1986; Hendriks and van Bergen, 1992; Firoozabadi and Pan, 2002; Okuno et al., 2010) have been developed. Another interesting approach is the so-called ‘shadow region’ method (Rasmussen et al., 2006) for bypassing some phase-stability tests during a simulation. It has been shown that both the reduced variables and ‘shadow region’ strategies reduce the computational time of the phase-stability tests significantly. Pan and Tchelepi (2011) combined phase-stability and bypassing using reduced variables, and they demonstrated that the combined strategy is very effective in reducing the overall cost of EoS computations.

One of the key concepts in compositional simulation is that of a tie-line, which is defined as a line that connects equilibrium phase compositions on the bubble- and dew-point curves for a given overall composition, \( z \). Any composition that lies on the tie-line forms a two-phase mixture. A set of tie-lines describes the two-phase space for a given pressure and temperature. The generalization of the tie-line for three-phase systems is the tie-triangle, which is a triangle that connects all three equilibrium
phase compositions for a given \((P, T, z)\). A set of tie-triangles describes the three-phase space for fixed \(P\) and \(T\). For an arbitrary number of phases, the object that describes the phase space is a tie-simplex, where a simplex is a generalization of the notion of a triangle.

A general approach for phase-behavior representation of two-phase compositional systems, based on the tie-line concept, was suggested by Entov et al. (2001). Their method involves the projection of the original compositional problem into the tie-line \((\Gamma)\) space, where simple polynomial approximations of the \(\Gamma\) space are used to capture the important features of the two-phase region (Voskov, 2002). Later, Voskov and Tchelepi (2009b) showed that linear interpolation in the discretized tie-line space can be used to represent the thermodynamic phase-behavior, which they refer to as Compositional Space Parameterization (CSP) based flow simulation. The original CSP approach is based on parameterizing the entire compositional space. It was shown that for purely hyperbolic 1D problems, projection of the solution into the tie-line space is invariant with respect to the hydrodynamic parameters of the problem (Entov, 1997; Voskov and Entov, 2001). Later, it was demonstrated (Voskov and Tchelepi, 2009a) that for compressible, multi-dimensional displacements in porous media, projection of the solution in the tie-line space is nearly invariant (i.e., the solution is spread around the 1D invariant path). By construction, the approach proposed by Voskov and Tchelepi (2009b) requires a-priori parametrization of the entire compositional space, which complicates the use of the approach for general-purpose compositional simulation.

The CSP ideas motivated the development of the Compositional Space Adaptive Tabulation (CSAT) method (Voskov and Tchelepi, 2008, 2009a). The CSAT method is based on the fact that gas-injection displacement processes involve a limited number of (key) tie-lines (Orr, 2007). The CSAT adaptively stores discrete tie-lines during a simulation. The collected tie-lines are used to look-up the phase-state of a mixture, thus replacing conventional phase-stability tests. Moreover, the tie-line compositional information can be used as an initial guess to accelerate standard flash computations. CSAT uses a discrete representation of specific regions of the compositional space associated with the solution route followed by the numerical simulator. CSAT is adaptive by construction; as a result, a standard EoS solver is still needed whenever
new regions of the compositional space are encountered by the simulation.

In this work, we generalize the Compositional Space Parameterization approach, and introduce a new framework for multiphase compositional simulation. This framework allows for continuous representation of the phase envelope as a function of composition, pressure, and temperature. The governing flow equations are discretized directly in tie-line space. In order to obtain the phase compositions, interpolation is used for points that lie inside a given discretization cell. We show that the errors associated with the interpolation are bounded and decrease with grid refinement (in \( \Gamma \)-space). This allows for the use of a limited number of tie-lines for accurate representation of a phase envelope. Within the CSP framework, we also develop a method that performs interpolation of all thermodynamic properties in the discretized tie-line space. This method allows for multilinear and continuous representation of the thermodynamic dependencies, and that facilitates systematic analysis of the coupling between the mass conservation laws and the thermodynamic constraints. The applicability of the generalized CSP method is demonstrated for several miscible and immiscible gas injection problems.

The proposed CSP framework serves as a new thermodynamically consistent approximation for general-purpose compositional simulation.

1.2 Three-Phase Thermal Simulation

Thermal compositional simulation is needed to model EOR processes, such as steam flooding, Steam-Assisted Gravity Drainage (SAGD), and Expanding Solvent-SAGD (ES-SAGD) (Nasr and Isaacs, 2001). As in the case of two-phase compositional modeling, thermal models are described by a system of nonlinear partial differential equations that include mass conservation and thermodynamic equilibrium constraints. However, since thermal effects are important here, the governing equations are coupled to the energy conservation equation.

Similar to isothermal simulation, the two common variable sets are the Natural Variables (Coats, 1978; Chien et al., 1989) and the Molar variables (Mifflin et al., 1991; Liu et al., 2009). An important difference between the two formulations, in the context of thermal modeling, is how temperature is treated. In the case of the Natural
Variables formulation temperature is treated as a primary unknown; whereas, in the Molar Variables formulation the total enthalpy is considered as a primary unknown instead of temperature. This difference in the primary variables results in different treatments of the phase-behavior computations. Specifically, an isobaric, isothermal (PT) flash is used in the Natural Variables approach, and an isobaric, isenthalpic (PH) flash is used in the Molar variables formulation. These two formulations result in different convergence properties for the set of governing nonlinear equations; however, it is still not clear which of the formulations is preferred in the general case.

Thermal compositional simulation is typically much more challenging compared with isothermal simulation. A major reason for the difficulties associated with thermal modeling is the tight coupling between pressure, temperature and saturations. Two well-known problems associated with this coupling are the so-called ‘narrow-boiling point’ problem (Chien et al., 1989) and the ‘apparent negative compressibility’ effect (Coats, 1980b). Both of these challenging problems are specific to thermal modeling. They impose significant nonlinear convergence issues during reservoir simulation regardless of the chosen variables formulation.

During a flow simulation, it is necessary to determine thermodynamic conditions in every gridblock, which includes determining of the number of phases present and obtaining the phase compositions. A conventional approach for these phase-behavior computations is the use of tables of precomputed K-values. As opposed to isothermal modeling, the K-values must be tabulated with respect to both pressure and temperature. K-values-based phase-behavior computations are attractive, since phase-stability testing in this case is non-iterative. This approach is the standard in current industrial reservoir simulators (CMG STARS, 2009; Schlumberger Eclipse, 2000).

Another approach for phase-equilibrium modeling for thermal simulation is the use of an EoS model (Varavei and Sepehrnoori, 2009; Iranshahr, 2012; Heidari, 2014; Zaydullin et al., 2014b). The rational for using an EoS-based approach instead of a K-values method is the possible loss of accuracy in the phase-behavior representation due to the restrictive assumptions of compositional independence of the K-values method. We note that several interesting methods have been introduced to improve the K-values representation by including limited dependence of the K-values on composition (Rannou et al., 2013; CMG STARS, 2009). The method introduced by Rannou et al.
(2013) employs interpolation of the K-values based on a single parameter that defines the invariant solution path obtained from solutions of hyperbolic problems computed in a preprocessing step. The method improves the phase-behavior representation accuracy for two-phase K-values-based modeling. However, it is not clear how this method can be generalized to thermal, three-phase flows. The method used in CMG STARS (2009) is based on using Hand’s tie-line interpolation, but the method also has limited applicability for systems that consist of four or more components.

While EoS-based modeling does not suffer from the limitations of the K-value approach, it is considerably more expensive for thermal simulation compared with the isothermal case. This is because the water phase must be included in the EoS description. In other words, EoS modeling with mass transfer among three fluid phases is required. As a result of having an additional (aqueous) phase, a large number of phase-state combinations (seven combinations) must be considered in the EoS description for a given multicomponent fluid system. The large number of phase combinations leads to increased computational cost of phase-stability testing and flash computations. Therefore, it is important to understand how the differences in the phase-behavior representation for the K-values and EoS-based approaches impact the modeling results.

Several authors compared simulation results obtained with the K-values and the EoS-based methods (Varavei and Sepehrnoori, 2009; Heidari, 2014). These authors found that the simulation results for the two methods can be quite different. However, in our opinion, the analysis of the problem presented in Varavei and Sepehrnoori (2009); Heidari (2014) does not provide a clear reasoning for this difference. For example, Varavei and Sepehrnoori (2009) associated the discrepancy in simulation results with the solubility of the water component in the resident oil. However, this solubility was not included in their K-values tables representation. Heidari (2014), on the other hand, provided consistent comparisons of the two methods, but he used complicated ES-SAGD examples, which are hard to analyze. In our study, instead of focusing on complex EOR processes, such as ES-SAGD, we perform the investigations using a very simple setting of one-dimensional steam and steam-solvent injection processes. We believe, this simple setting allows for a better understanding of the underlying interplay between the displacement and the phase-behavior.
1.3 Three-Phase Simulation: Bypassing Strategies

For a wide range of problems of practical interest, it is usually adequate to assume that only two hydrocarbon fluid phases (i.e., oil and gas) can coexist at equilibrium. This class of problems includes most gas-injection processes, Water Alternating Gas (WAG) injection, and production from gas-condensate reservoirs. However, the two-phase assumption can be inadequate for modeling some EOR processes, such as steam-solvent coinjection where the interactions between water and hydrocarbon components can play an important role. Another example of a displacement process where three-phase EoS modeling is necessary is cold CO$_2$ injection, where a third CO$_2$-rich liquid-phase can form at low temperatures. In our experience, for low-temperature CO$_2$ injection problems, the assumption of only two hydrocarbon phases can lead to substantial nonlinear convergence issues, or even, to non-convergent behavior. Also, this type of problem cannot be modeled using the three-phase K-values method, since the displacement is near-miscible. Therefore, there is a clear need for three-phase EoS modeling for such processes. We also note that specifically for the low-temperature CO$_2$ injection problems, the phase labeling by itself can be challenging, even when a three-phase EoS model is employed (Xu and Okuno, 2015).

As mentioned earlier, three-phase EoS-based modeling can be substantially more expensive compared with two-phase simulation. In this work, we present a novel strategy for the bypassing of phase-state identification that can be used in multicomponent, multiphase thermal-compositional simulation. The method makes use of the ideas developed in the Compositional Space Parameterization approach. Our ‘bypass’ method uses information from the parameterized extensions of the ‘key’ tie-simplexes (tie-triangles for the three-phase systems). The parameterization is performed in the discrete phase-fraction space. In this space, the phase fractions can be negative, or greater than unity; this allows for parameterization of the plane that corresponds to a tie-simplex extension. Once the tie-simplex extensions are discretized, a standard three-phase flash is used adaptively to compute the phase-states at the discrete points in the compositional space. If all discretization vertices for a given discrete cell that lie on the plane have the same phase state, then this state is assigned to the entire computational cell, and flash calculations are bypassed for the compositions of that cell. Here, we make use of the continuity of the tie-simplex parameterization, which
was proven in the earlier work of Iranshahr (2012).

As in the case of CSP-based modeling of two-phase displacements, one of the advantages of the proposed bypass method is its independence on the actual EoS model used. It is known, for example, that the classical cubic Equations of States, such as Peng-Robinson (Peng and Robinson, 1976) and Soave-Redlich-Kwong (Soave, 1972), can be inadequate in the representation of polar components (e.g., water). Therefore, these classical EoS models may not be an optimal choice for thermal modeling. On the other hand, the more advanced EoS models, such as Statistical Associating Fluid Theory (SAFT) EoS (Chapman et al., 1989), can be more accurate for this type of simulation, but also substantially more expensive computationally. Therefore, our new bypass method can be advantageous for cases when advanced EoS models are used.

The three-phase bypass method can be viewed as an extension of the CSP framework for multicomponent systems that can form three or more phases. We note, however, that our new method allows for skipping of the unnecessary phase-identification computation only and does not replace the flash computations. Therefore, the bypass method is only a partial extension of the general CSP framework for the case of three-phase simulation.

1.4 Thesis overview and contributions

We highlight three main contributions of this work compared with the existing literature on compositional reservoir simulation.

The first contribution is the development of a general Compositional Space Parameterization framework for two-phase compositional simulation. Chapter 2 summarizes the framework components, such as the variables formulation, interpolation, and discretization techniques, and treatment of miscibility. A set of examples, which mimic real-field scenarios, is presented at the end of the chapter. We close the chapter with a discussion on the possible use and extension of the framework for more challenging problems.

The second contribution, which is described in Chapter 3, is related to the analysis
of the impact of the K-values method assumptions on the results of thermal compositional simulation. Chapter 3 briefly describes the governing equations for thermal reservoir simulation, as well as two methods for the phase-behavior representation. Namely, we focus on K-values and EoS models. The rest of the chapter presents detailed numerical analysis and discussion of the impact of using K-value tables for phase equilibrium computations.

The third contribution is a new bypass method for fast phase-state identification associated with three (and more) phases. The method is described in Chapter 4. We start the chapter by highlighting specific aspects and ideas of the Compositional Space Adaptive Tabulation method (CSAT). We next proceed with a detailed description of the phase-identification bypass method. Next, we demonstrate the approach using examples of steam-solvent and low temperature CO$_2$ injection. We finish the chapter with a short discussion on the applicability of the bypass method for more challenging problems.

We present our conclusions and future work in Chapter 5.
Chapter 2

Compositional Space
Parameterization for two-phase displacements

2.1 Conventional approach for compositional flow simulation

The system of equations for two-phase isothermal compositional reservoir simulation can be written as:

\[
\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{2} x_{i,j} \rho_j \, S_j \right) - \text{div} \sum_{j=1}^{2} x_{i,j} \rho_j \left( k \frac{k_{rj}}{\mu_j} \nabla P \right) + \sum_{j=1}^{2} x_{i,j} \rho_j g_j = 0, \quad i = 1, \ldots, n_c.
\]  

(2.1)

Here, \( x_{i,j} \) is the concentration of component \( i \) in phase \( j \), \( S_j \) is phase saturation, \( \rho_j \) is the phase molar density, \( k \) is permeability, \( k_{rj} \) is relative permeability, \( \mu_j \) is the phase viscosity and \( P \) is pressure. Capillary pressure, chemical reactions, and diffusion are neglected in this research.

Instantaneous thermodynamic equilibrium is the usual assumption for the compositional model and can be expressed as equality of fugacities in the vapor and liquid.
phases:

\[
f_{i,o}(P, T, x_o) - f_{i,g}(P, T, x_g) = 0, \quad i = 1, \ldots, n_c. \tag{2.2}
\]

Here, \( f_{i,g} \) and \( f_{i,o} \) represent the fugacity of component \( i \) in the vapor and liquid phases, respectively. We use the following standard expression for phase fugacities (see, for example, Firoozabadi (1999)):

\[
f_{i,j}(P) = \frac{\exp\left(\frac{b_i(Z - 1)}{b}ight)}{(Z - B)} \exp\left(\frac{A}{B\sqrt{u^2 - 4w}} \left(\frac{b_i}{b} - \delta_i\right) \ln\left(\frac{2Z + B(u + \sqrt{u^2 - 4w})}{2Z + B(u - \sqrt{u^2 - 4w})}\right)\right). \tag{2.3}
\]

Here, \( u, w, A, \) and \( B \) are parameter values for a cubic equation of state, and \( Z \) is the compressibility factor. The thermodynamic relations are usually addressed by using one of two strategies:

- Solve the thermodynamic constraints together with the mass conservation flow equations (2.1).
- Solve the thermodynamic equilibrium equations separately and couple them with the mass conservation equations in a two-step approach.

Each of these approaches has its own advantages and drawbacks (Voskov and Tchelepi, 2012).

The overall composition, \( z_i \), for a two-phase system can be represented as a linear combination of phase compositions \( x_{i,j} \):

\[
z_i - x_{i,o}L + x_{i,g}(1 - L) = 0, \quad i = 1, \ldots, n_c, \tag{2.4}
\]

\[
\sum_{i=1}^{n_c}(x_{i,o} - x_{i,g}) = 0. \tag{2.5}
\]

where \( L \) is the fraction of the liquid (oil) phase.

The fully implicit method (FIM) is used to discretize the system of equations (2.1) in time for a given set of unknowns. The space discretization is performed using the two-point flux approximation (TPFA) and single-point, phase-based, upstream
2.1. CONVENTIONAL APPROACH

weighting (Aziz and Settari, 1979; Peaceman, 1977). The resulting system of nonlinear
equations is then solved using the Newton-Raphson method, in which a Jacobian
system is assembled and solved for each nonlinear (Newton) iteration.

In two-phase compositional simulations, a mixture $\mathbf{z}$ at a given $P$ and $T$ in any
gridblock can be in a single (vapor, or liquid), or two-phase state. The phase equilib-
rium computations differ depending on the state of the system. Namely, the phase
stability test (Michelsen, 82a) is typically used for single-phase mixtures, in order to
identify whether the mixture can split into two-phases. If a mixture is identified as
unstable (two-phase state), a flash calculation algorithm (Michelsen, 82b) is used to
obtain the phase compositions. Depending on the nonlinear formulation used, the
flash calculations may be necessary for all of the gridblocks that have a two-phase
state. Hence, the phase equilibrium computations usually involve a two-step proce-
dure:

- For any gridblock in which a single phase is present, the phase stability test is
performe\big to check whether the current state will switch to a different single-
phase or to a two-phase state.

- If the mixture is not stable, flash calculations are performed to compute the
phase compositions at equilibrium. The flash procedure is represented as a so-
lution of Eqs. (2.2)-(2.5). The solution of this system usually involves the com-
bination of Successive Substitution Iterations (SSI) and the Newton method.

2.1.1 Nonlinear formulations

It can be shown (Cao, 2002) that the coupled system of equations (2.1 - 2.5) can be
reduced to a system of $n_c$ primary equations with $n_c$ primary unknowns (variables).
The remaining secondary unknowns can be obtained from the primary variables and
the secondary equations. Thus, different sets of primary and secondary unknowns
can be used for compositional flow simulation. In this work, Natural (Coats, 1980a)
and Molar (Chien et al., 1985; Collins et al., 1992) Variables were used to perform
the conventional compositional simulations.

1. **The Natural Variables** formulation employs the following set of unknowns
for two-phase gridblocks (number of unknowns is indicated in square brackets):
• $P$ – pressure [1],
• $S_g$ – phase saturations [1],
• $x_{i,j}$ – phase compositions [$2n_c$],

Here, the overall composition $z$ can be obtained from (2.4). For the single-phase gridblocks, the unknowns are:

• $P$ – pressure [1],
• $z_i$ – overall compositions [$n_c$],

For this formulation, the system of equations (2.1) is chosen as the primary equation set. The primary unknowns for the two-phase gridblocks are $P$, $S_g$, and $n_c - 2$ phase compositions, $x_{i,g}$. The remaining $n_c + 2$ phase compositions are treated as secondary variables (Cao, 2002). The phase equilibrium computations for this formulation are performed as follows: 1) the phase stability test is used to identify whether a single-phase gridblock can switch its state, 2) the fugacity constraints (2.2) for two-phase gridblocks are resolved along with the primary equations (2.1) within the global Newton loop. The flash algorithm for this formulation is only used to obtain the phase compositions in the case of phase appearance, which is detected by stability testing (Cao, 2002). We also note, however, that the fugacity constraint (2.2) equations can be resolved using the flash algorithm locally prior to the global Newton iteration.

2. **The Molar Variables.** For this formulation, the following primary unknowns are used:

• $P$ – pressure [1],
• $z_i$ – overall composition [$n_c$],

Here, similarly to the Natural Variables, the phase stability test is used for all single-phase gridblocks. If a two-phase state is detected, flash computations must be performed to obtain the phase compositions for this gridblock. Importantly, the flash computations step cannot be skipped here. This is a major point of difference between the Molar Variables and Natural Variables.
formulations. The flash computations are necessary when using Molar Variables formulation, because of the need for derivatives of phase compositions, $x_{i,j}$, with respect to the primary unknowns, $z_i$. These derivatives are obtained using the implicit function theorem equation (Voskov and Tchelepi, 2012), namely:

$$\frac{\partial x_{i,j}}{\partial z_i} = \frac{\partial F}{\partial z_i} \left( \frac{\partial F}{\partial x_{i,j}} \right)^{-1},$$

(2.6)

where $F$ represents the system of fugacity equations (2.2) along with the constraints (2.4, 2.5).

### 2.2 Γ-Variables Formulation

As discussed in the previous section, for a given overall composition, $z$, one can find the corresponding phase compositions in the vapor and liquid phases, $x_{i,j}$, by performing a two-phase flash. A line that connects compositions on the bubble- and dew-point curves is called a tie-line. Here, we assume that tie-lines never intersect inside the compositional space. This assumption is valid for the vast majority of reservoir fluids that do not contain extremely heavy components, and, therefore, the assumption is not restrictive for the two-phase compositional systems of practical interest.

Since the tie-lines do not intersect inside the compositional space, each tie-line can be uniquely parameterized by a $\gamma$ parameter that is constant along the tie-line. The set of these parameters forms the Γ-space (tie-line space). Here, $\gamma$ is defined as a set of coordinates associated with the center point of the tie-line (Entov et al., 2001). In fact, the $\gamma$-parameter can be selected as any point along the tie-line; for example, $\gamma$ can be defined as a linear combination of the phase compositions (i.e., $\gamma_i = \alpha x_{i,o} + (1 - \alpha) y_{i,o}$). Regardless of the exact definition of the $\gamma$-parameter, each tie-line in the compositional space has a corresponding unique $\gamma$ in the Γ-space. The dimension of the parameterized space depends on the number of components and phases. For a two-phase system, it is equal to $[n_c - 2]$. In the general case the dimension of the Γ-space is equal to $[n_c - n_p]$.

Voskov and Tchelepi (2009a) proposed an approach for fast phase-equilibrium
computations based on $\gamma$-parameterization of the compositional space using the \{\(P, z\)\} variables set. This approach allows for efficient interpolation of the phase compositions, \(x_{i,j}\), using information from the discretized (tessellated) \(\Gamma\)-space. However, the approach relies on the assumption that (2.2) is linear within any simplex of the discretized space. This linearity assumption requires very small simplexes leading to an excessively large number of simplexes to cover the entire compositional space. Moreover, due to the assumption of linearity of (2.2), the saturation field obtained with large (coarse) simplexes may display non-physical oscillations (Zaydullin et al., 2010).

Figure 2.1 shows a typical 1D saturation profile (immiscible gas injection) for a four-component mixture obtained with the original $\gamma$-parameterization and conventional approaches. It can be seen that the saturation profile is oscillatory for the case where parameterization is used, whereas a monotonic profile is observed for the case of the conventional method.

![Figure 2.1: Saturation distribution for a four component system \{\(C_1, C_{10}, C_4, CO_2\)\} using large (a) and small (b) simplexes; EoS-based solution is represented by the solid line, $\gamma$-parameterization solution in circles.](image)

In order to overcome the limitations of the Voskov and Tchelepi (2009a) approach, we propose a new formulation, which is based on the $\gamma$-parameters. The new variables set is \(\{P, L, \gamma_i, i = 1, \ldots, n_c - 2\}\), where \(L\) is liquid fraction. We refer to this as a
2.3. **COMPOSITIONAL SPACE PARAMETERIZATION (CSP)**

Γ-Variables set. Since the γ-parameters are used directly as the nonlinear unknowns (instead of z), the proposed variables set does not require the linearity assumption discussed earlier. However, the Γ-Variables set requires a special treatment of the phase equilibrium computations; that is, given \{P, L, \gamma_i, i = 1, \ldots, n_c - 2\}, one needs to reconstruct the phase compositions and all the necessary derivatives. These special phase-equilibrium computations can be performed in two different ways:

- Given \{P, \gamma_i, i = 1, \ldots, n_c - 2\}, flash calculations in the parameterized space can be used to obtain the phase compositions and related derivatives. This specialized γ-based flash algorithm is discussed later in the chapter. This approach makes the Γ-Variables set similar to the Natural Variables formulation with the locally resolved fugacity constraints (2.2).

- Given \{P, \gamma_i, i = 1, \ldots, n_c - 2\}, the phase compositions can be obtained by interpolation in the discretized Γ-space. We refer to this approach as Compositional Space Parameterization (CSP) for two-phase simulation. The rest of the chapter is dedicated to the description of this new parameterization approach.

### 2.3 Compositional Space Parameterization (CSP)

Based on the Γ-Variables set, a new algorithm for phase equilibrium computations is introduced. Given the tie-line parameters, γ, pressure, and temperature, the proposed phase equilibrium procedure returns the liquid and vapor phase compositions and all the necessary derivatives. The algorithm is based on adaptive discretization of the tie-line space and subsequent interpolation of the phase compositions as a function of the γ-parameter. The pressure (and possibly temperature) dependencies of the phase compositions are also captured through linear interpolation.

The algorithm is as follows:

1. For each pressure in the interval of interest, the phase diagram is adaptively constructed in the parameterized space.

2. The Γ-space is tessellated based on the supporting γ points (tessellation vertices).
3. For any given \( \{P, \gamma\} \), the phase compositions for the end-points of the pressure interval \([P_j, P_{j+1}]\) are computed using interpolation inside the simplex.

4. The phase compositions are obtained by linear interpolation in the pressure interval \( P \in [P_j, P_{j+1}] \).

Each of these steps is discussed in detail below.

### 2.3.1 Interpolation in parameterized space

Since a tie-line is a continuous function of \( P, T \) and composition \( z \) (Iranshahr et al., 2009b), linear interpolation can be used to construct a tie-line inside a simplex for the pressure interval. The interpolation algorithm was originally proposed by Voskov and Tchelepi (2009b) for the standard compositional variables set \( \{P, z\} \). The original algorithm was modified in order to use the \( \Gamma \)-Variables for the representation of the compositional space (Zaydullin et al., 2012).

To represent a tie-line as a function of the parameter \( \gamma \), the \( n \)-dimensional \((n = n_c - 2)\) \( \Gamma \)-space is discretized into simplexes using a triangulation technique (e.g., Delaunay triangulation). Next, for any point inside a discretization cell (simplex), barycentric (Sibson, 1981) interpolation is performed. The interpolation coefficients (barycentric coordinates) are determined by solving the following system of linear equations:

\[
\gamma_i = \sum_{k=1}^{n+1} \beta_k \gamma_{k,i}^*, \quad i = 1, \ldots, n
\]  

(2.7)

where the \( \beta_k \) denote the barycenter coordinates of each vertex of a simplex \((n + 1\) vertices in \( n \)-dimensional space), \( \gamma_{k,i}^* \) are the coordinates of the \( k^{th} \) vertex. Here, we look for the barycenter coordinates, \( \beta_k \), for a given value of \( \gamma \) and fixed coordinates of simplex nodes, \( \gamma_{k}^* \). The system of linear equations (2.7) can be rewritten in matrix notation as follows:

\[
\begin{bmatrix}
\Gamma \\
e
\end{bmatrix}
\begin{bmatrix}
\beta \\
1
\end{bmatrix} =
\begin{bmatrix}
\gamma \\
1
\end{bmatrix},
\]  

(2.8)
where, $\mathbf{\Gamma}$ is a matrix of the coordinates of the $(n+1)$ vertices, and $\mathbf{e}$ is the unit vector, which arises from the constraint on the sum of the barycenter coordinates.

By solving the linear system (2.8), one can determine the barycenter coordinates of the interpolated point. Since the matrix $\mathbf{\Gamma}$ does not depend on the coordinates of the interpolated point, the barycenter coordinates are linear functions of the tie-parameter $\gamma$.

Knowing the barycenter coordinates of the interpolated point, the phase compositions for the end-points for the pressure interval of interest can be computed as follows:

$$x_{i,j}^1 = \sum_{k=1}^{n+1} \left(x_{i,j}^*(P_1)\right)_k \beta_k, \quad i = 1, \ldots, n_c \quad j = \{o,g\}, \quad (2.9)$$

$$x_{i,j}^2 = \sum_{k=1}^{n+1} \left(x_{i,j}^*(P_2)\right)_k \beta_k, \quad i = 1, \ldots, n_c \quad j = \{o,g\}, \quad (2.10)$$

where $(x_{i,j}^*)_k$ denote the phase compositions that correspond to $\gamma_k^*$. The next step is a linear interpolation of the phase compositions for the pressure interval:

$$x_{i,j} = \pi(P)x_{i,j}^1 + (1 - \pi(P))x_{i,j}^2 \quad i = 1, \ldots, n_c \quad j = \{o,g\}, \quad (2.11)$$

where $\pi(P)$ is the interpolation coefficient in pressure. Since linear interpolation in both pressure and composition is used computation of the phase compositions, the derivatives of all the interpolation coefficients $\beta_i(\gamma)$ and $\pi(P)$ are constant:

$$\frac{\partial \beta_i}{\partial \gamma} = \text{const}, \quad i = 1, \ldots, n+1, \quad j = 1, \ldots, n \quad (2.12)$$

$$\frac{\partial \pi(P)}{\partial P} = \text{const}. \quad (2.13)$$

Equations (2.9-2.11) indicate that the proposed interpolation allows for decoupling of the elliptic ($P$) and hyperbolic ($\gamma$) dependencies of the phase compositions, $x_{i,j}$.

Since the CSP method is based on piece-wise linear interpolation in the tie-simplex space, the first derivative of the phase compositions, $x_{i,j}$, is discontinuous on the boundary of each simplex. These discontinuities may lead to oscillations between two
adjacent simplexes; however, we do not observe this problem even with challenging miscible displacements. This is because the variables change between two adjacent simplexes associated with non-tie-line solution paths are typically smoother compared to those of tie-line paths.

2.3.2 Discretization of the tie-line space

Voskov and Tchelepi (2009a) proposed an algorithm for $\Gamma-$space discretization based on a Delaunay triangulation. In their approach, the $\Gamma-$space is discretized in a pre-processing stage, which can lead to large numbers of supporting points as the number of components increases. Here, we propose an adaptive procedure for the tie-line space discretization. The procedure is based on generalization of the octree data structure.

An octree is a data structure in which each node has exactly eight children (Eberhardt et al., 2010). The two-dimensional analog of an octree is a quadtree – a tree data structure in which each node has exactly four children. Two major advantages of the octree-based approach are: 1) good memory efficiency because the size of the tree is limited, and 2) fast search. These advantages make an octree structure attractive for our adaptive interpolation. Since the dimension of the $\Gamma$-space can be greater than three, we generalized the octree data structure for spaces of arbitrary dimension. Next, each hyper-cube (see Figure 2.2) is further triangulated using the Delaunay method. This additional step is needed in order to use a relatively inexpensive barycentric interpolation. Using the barycentric interpolation is especially important for cases when the number of components is large, since it requires only $n_c - 1$ vertices for the interpolation. Also, since the Delaunay method is used to triangulate cubes of the same dimension ($n_c - 2$), the triangulation is performed once only in a pre-processing stage; the tessellation is stored and used for all hyper-cubes. The advantages of the proposed algorithm can be summarized as follows:

- The barycentric interpolation requires only $n_c - 1$ supporting points, whereas polylinear interpolation (generalization of trilinear interpolation) involves $2^{n_c-1}$ supporting vertexes for interpolation. Hence, the number of supporting points becomes substantial for the case of polylinear interpolation when the number of
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components is larger than four. Therefore, barycentric interpolation is preferred for general-purpose simulation.

• The algorithm allows for construction of regular simplexes.

• Delaunay triangulation needs to be performed once only, since each hyper-cube has the same triangulation pattern.

Figure 2.2 depicts a typical discretized tie-simplex space for a five-component system. The dimension of the space in this case is three. Here, adaptive refinement of the octree is used to increase interpolation accuracy of phase compositions. The green dots represent the interpolated points, and the red dots are the supporting points. Each hyper-cube is triangulated using the Delaunay method.

Although adaptive refinement has not been thoroughly investigated in this research, it is evident that refinement in \( \Gamma \)-space can be used to reduce the interpolation error. One possible criterion for the refinement is the nonlinearity of the solution path in the \( \Gamma \)-space, which can be identified by tracking the solution path gradients. Additional settings where adaptive refinement can be useful include compositional problems with large numbers of components. In such cases, a large portion of the solution path may lie areas close to the \( \Gamma \)-space boundary, making finer grids desirable in such regions.

![Figure 2.2: Example of a tessellated octree.](image-url)
The computational cost of the proposed CSP algorithm depends on the number of components in the modeled system. Figure 2.3 compares the approximate number of arithmetic operations required to obtain \( n_c n_p \) phase compositions for the CSP methods against those of the conventional flash algorithm. For this comparison, we assumed that the computational cost of multiplication, division, and addition operations are the same. Also, for the conventional flash algorithm, we assumed that small number of Successive Substitution Iterations (SSI) is adequate for convergence. As shown in Figure 2.3, the number of operations increases linearly with the number of components for the conventional SSI flash; the slope of the number of operations curve is proportional to the number of SSI iterations. For the case of the CSP method, the number of operation required for the interpolation is substantially lower than the conventional flash when the number of components is less than ten. However, due to the requirement to search within the triangulated tie-line space, the number of operations increase quadratically when large number of components are present. We note that the number of operations for the CSP method is estimated assuming that the search within the triangulated space needs to be performed for random values of the \( \gamma \)-parameters. However, during the actual reservoir simulation, the computational cost of a simplex search within the triangulated tie-line space will be less dominant since the values of the \( \gamma \)-parameters do not change abruptly.

### 2.3.3 Flash calculation in parameterized space

In order to build the supporting points in the tie-line space, the phase compositions for a given \( P, T \), and tie-line parameter \( \gamma \) must be determined. For this purpose, a new flash calculation algorithm in the parameterized \( \Gamma \)-space is proposed.

The system of nonlinear equations to be solved in \( \Gamma \)-space can be written as

\[
\gamma_i - g_i(x_o, x_g) = 0, \quad i = 1, \ldots, n_c - 2 \tag{2.14}
\]

\[
f_i,o(P, T, x_o) - f_i,g(P, T, x_g) = 0, \quad i = 1, \ldots, n_c. \tag{2.15}
\]

\[
\sum_{i=1}^{n_c} x_{i,j} - 1 = 0, \quad j = o, g. \tag{2.16}
\]

The definition of \( g_i \) depends on how one determines \( \gamma_i \). Here, the center point of the
2.3. COMPOSITIONAL SPACE PARAMETERIZATION (CSP)

Figure 2.3: Comparison of the approximate number of arithmetic operations for conventional flash and the CSP method.
tie-line is used as the tie-line parameter, i.e., \( g_i = \frac{(x_{i,o} + x_{i,g})}{2}, \ i = 1, \ldots, n_c - 2 \). Thus, for given \( P, T \) and \( \gamma \), the corresponding \( x_o \) and \( x_g \) are needed.

Similar to the standard flash procedure, the algorithm starts from the phase relations provided by Wilson’s equation

\[
K_i = \frac{x_{i,g}}{x_{i,o}} = \frac{P_{c,i}}{P} \exp \left( 5.37(1 + w_i) \left( 1 - \frac{T_c}{T} \right) \right), \ \forall i = 1, \ldots, n_c.
\]

Here, \( P_c \) and \( T_c \) are the critical pressure and temperature, and \( w_i \) is the acentric factor. With the \( K \)-values and \( \gamma \) parameters known, \( 2n_c - 4 \) phase compositions can be calculated:

\[
x_{i,o} = \frac{2\gamma_i}{K_i + 1}, \ \forall i = 1, \ldots, n_c - 2,
\]

\[
x_{i,g} = K_i x_{i,o}, \ \forall i = 1, \ldots, n_c - 2.
\]

Next, the remaining mole fractions (i.e., \( x_{i,j}, \ i = \{n_c-1, n_c\}, \ j = \{o, g\} \)) need to be computed.

From the definition of the \( K \)-values, we have:

\[
(K_{n_c-1} - K_n) x_{n_c,o} = K_{n_c-1} x_{n_c,o} - K_{n_c} x_{n_c,o} = K_{n_c-1} x_{n_c,o} - x_{n_c,g},
\]

which can be rearranged as:

\[
K_{n_c-1} x_{n_c,o} - x_{n_c,g} = (K_{n_c-1} x_{n_c,o} + x_{n_c-1,g}) - x_{n_c-1,g} - x_{n_c,g}
\]

\[
= K_{n_c-1} (x_{n_c,o} + x_{n_c-1,g}) - x_{n_c-1,g} - x_{n_c,g}.
\]

Considering equation (2.16), the last relation can be written as:

\[
K_{n_c-1} x_{n_c,o} - x_{n_c,g} = K_{n_c-1} \left( 1 - \sum_{i=1}^{n_c-2} x_{i,o} \right) + \sum_{i=1}^{n_c-2} x_{i,g} - 1.
\]
Combining (2.20) and (2.22) leads to:

\[
x_{n_c,o} = \frac{\sum_{i=1}^{n_c-2} x_{i,g} + K_{n_c-1} \left( 1 - \sum_{i=1}^{n_c-2} x_{i,o} \right) - 1}{K_{n_c-1} - K_{n_c}}.
\]  

(2.23)

The other compositions can be found from (2.16) and the K-value definition. Next, the \(x_{i,j}\) are substituted into the fugacities, Eq.(2.15), and the \(K\)-values are updated as follows:

\[
K^{(m)}_i = \frac{K^{(m-1)}_i f_{i,o}^{m-1}}{f_{i,g}^{m-1}},
\]

(2.24)

where \(m\) is the SSI iteration number, and \(\Phi_i\) is the fugacity coefficient of component \(i\). Note that the SSI flash does not require solution of the Rachford-Rice equation (Rachford and Rice, 1952).

The SSI iterations are repeated until the desired tolerance of the residual is achieved. Then, the algorithm switches to the Newton method. Such an approach requires linearization of the system (2.14)-(2.16) for each Newton iteration and updating of the nonlinear unknowns, \(x_o\) and \(x_g\), based on the solution of the linear system until convergence is reached.

2.3.4 Use of nonphysical phase compositions

The use of the generalized octree data structure and the \(\Gamma\)-Variables formulation requires tphase compositions for arbitrary values of the \(\gamma\) parameter. However, for a given pressure and temperature, it is possible to obtain a supporting \(\gamma\) point that corresponds to phase compositions that are not in the physical domain. Thus, the \(\gamma\)-based flash algorithm used for computations of the supporting points is extended for calculations in the non-physical compositional space (negative phase compositions).

The following modifications are introduced in the flash algorithm:

- Only positive phase compositions are allowed during the SSI process. Here we scale the negative compositions back to a small positive value. This approach allows us to converge the fugacity constraints equations (2.2) to any desired precision; however, the constraints (2.14) may be violated.
Once convergence of the fugacity constraints in the SSI process is achieved, we switch to the Newton method with a small damping factor. Namely, the Newton update vector is scaled such that the maximum change in the phase compositions during one iteration does not exceed 0.01. This safeguarded strategy allows for smooth convergence of the phase compositions in the non-physical region while satisfying all the residual equations (2.14-2.16). Obviously, the computational cost of such a safeguarded strategy can be substantial. However, our numerical experience suggests that nonphysical compositions occur quite rarely during the simulations.

The use of negative phase compositions may potentially lead to a 1) negative overall compositions, and 2) negative compressibility factors, \( Z \). Wang and Orr (1998) showed that a modified flash algorithm that can be used to calculate phase compositions for mixtures that lie outside the physical compositional space; however, here, the specified overall composition must lie on the extension of a tie-line. That is, the obtained phase compositions must lie in the physical domain. Our \( \gamma \)-based flash algorithm allows for both negative phase and negative overall compositions. We also note that by allowing nonphysical solutions of (2.14-2.16), we may still satisfy the physical restrictions in (2.4) with an appropriate choice of the phase fraction, \( L \).

The use of a negative compressibility factor, \( Z \), may lead to negative argument in the logarithm of Eq. (2.3). This difficulty can be overcome by using complex-valued logarithms. The use of nonphysical phase compositions and complex domain methods were proposed by Lucia et al. (1993). The authors suggested performing mathematically consistent flash calculations in the complex domain and showed that the use of complex compressibility and complex phase compositions improve the convergence rate of the flash process. Moreover, they showed calculations that permit compositions and K-values with negative real and imaginary parts.

Figure 2.4 displays the phase envelope calculated for a \( \{CO_2, NC_4, C_1, C_{10}\} \) mixture flashed at 130 bars and 372 K. The green surface represents the tie-line space. We can see that a portion of the phase envelope is outside the compositional space. However, the phase envelope is still changing continuously with the \( \gamma \) parameter.
We now present an estimate of the interpolation error in tie-line space. It can be proven using Rolle's theorem that the error associated with linear interpolation in pressure and liquid fraction is bounded by:

$$|R_i| < \frac{h}{8} \max_{x_1 < x < x_2} \left| f''(x) \right|,$$  \(2.25\)

where \(R_i\) is the error associated with interpolation of function \(f\), and \(h = |x_2 - x_1|\) is the discretization interval length.

The \(\gamma\) parameter is defined as the set of coordinates associated with the center point of the tie-line, i.e., \(\gamma_i = (x_{i,o} + x_{i,g})/2, i = 1 \ldots n_c - 2\) (Entov et al., 2001; Voskov, 2002). Using K-values \(K_i = x_{i,g}/x_{i,o}\), the \(\gamma\) parameter can be represented as

$$2\gamma_i = x_{i,o}(1 + K_i), \quad i = 1 \ldots n_c - 2.$$  \(2.26\)
For any given $\gamma$, we can find unique $n_c - 1$ real numbers $\beta_k$, such that

$$
\gamma_i = \sum_{k=1}^{n_c-1} \beta_k \gamma_i^k, \quad i = 1 \ldots n_c - 2
$$

(2.27)

$$
\sum_{k=1}^{n_c-1} \beta_k = 1,
$$

(2.28)

where $\gamma_k, \quad k = 1 \ldots n_c - 1$ are vectors of supporting points (vertices of a simplex). The real numbers, $\beta_k$, are called the barycentric coordinates of $\gamma$.

If we assume that the K-values are independent of composition (constant K-values), Eq.(2.26) represents a linear dependency of phase composition, $x_o$, on the $\gamma$ parameter. Therefore, by Taylor expansion, we can write:

$$
x_{i,o}(\gamma_k) = x_{i,o}(\gamma) + \nabla x_{i,o}(\gamma)(\gamma_k - \gamma), \quad i = 1 \ldots n_c - 2.
$$

(2.29)

Note that in the case of constant K-values, Eq.(2.29) is exact. Next, we follow the derivation scheme presented in (Chen, 2008). Multiplying both sides of (2.29) by the $\beta_k$ and summing over all $k$, we obtain:

$$
\sum_{k=1}^{n_c-1} \beta_k x_{i,o} = x_{i,o} \sum_{k=1}^{n_c-1} \beta_k + \nabla x_{i,o}(\sum_{k=1}^{n_c-1} \beta_k \gamma_k - \gamma \sum_{k=1}^{n_c-1} \beta_k), \quad i = 1 \ldots n_c - 2.
$$

(2.30)

By definition of barycentric coordinates $\sum_{k=1}^{n_c-1} \beta_k = 1$; therefore, Eq. (2.30) reduces to

$$
|R_{\gamma,i}| = \left| \sum_{k=1}^{n_c-1} \beta_k x_{i,o}(\gamma_k) - x_{i,o}(\gamma) \right| = 0, \quad i = 1 \ldots n_c - 2,
$$

(2.31)

where $|R_{\gamma,i}|$ represents the error associated with interpolation of phase compositions in the tie-line space.

Therefore, for the case of constant K-values, the barycentric interpolation is exact. Obviously, the error associated with interpolation of $x_{i,g}$ is also zero.

For the general case, the K-values depend on composition, so that the Taylor
2.4. **INTERPOLATION ERROR IN TIE-LINE SPACE**

series expansion of $x_{i,o}$ around $\gamma_k$ is

$$x_{i,o}(\gamma_k) = x_{i,o}(\gamma) + \nabla x_{i,o}(\gamma)(\gamma_k - \gamma) + \frac{1}{2}(\gamma_k - \gamma)^T \nabla^2 x_{i,o}(\gamma)(\gamma_k - \gamma) + \ldots \quad (2.32)$$

We now assume that we can neglect terms with order higher than two (i.e., $[\gamma_k - \gamma]^T[\gamma_k - \gamma]$ is small). After applying the same technique as in the case of constant K-values, we obtain the following error estimate:

$$\sum_{k=1}^{n_c-1} \beta_k x_{i,o}(\gamma_k) - x_{i,o}(\gamma) \approx \frac{1}{2} \sum_{i,j=1,j>1}^{n_c-1} \beta_i \beta_j (\gamma_i - \gamma_j)^T \nabla^2 x_{i,o}(\gamma)(\gamma_i - \gamma_j) \quad (2.33)$$

Next, using the Cauchy-Schwarz inequality and matrix norm properties, we obtain the following expression:

$$R_{\gamma,i} \leq \frac{1}{2} V_\gamma^2 \| \nabla^2 x_{i,o} \| \quad i = 1 \ldots n_c - 2, \quad (2.34)$$

where $V_\gamma = \max_{i,j} \| \gamma_i - \gamma_j \|$. A similar error estimation can be derived for the vapor compositions, $x_{i,g}$.

It is important to note that the estimate of Eq. (2.34) is obtained assuming weak dependence of the K-values on composition. However, this assumption is not valid in the vicinity of the critical point, where the higher order terms in the Taylor series (2.32) expansion cannot be neglected.

**Numerical examples**

We compare the phase envelopes obtained using CSP interpolation with those obtained using the conventional flash algorithm. The comparison is performed for two hydrocarbon mixtures, namely:

1. $\{CO_2, \ NC_4, \ C_1, \ C_8\}$.

2. $\{N_2, \ NC_4, \ C_1, \ C_8\}$.

Both mixtures are flashed at 100 bars and 372 K. As can be seen in Figures 2.5-2.6, the two systems exhibit very different phase behaviors. The presence of N$_2$ for
the mixture 2, leads to an almost linear phase envelope (approximately constant K-values); whereas for mixture 1, we can clearly observe the critical locus.

The CSP interpolation algorithm is performed using various levels of discretization, using a combination of quadtree and Delaunay triangulation (Zaydullin et al., 2012). The coarsest grid has $V_\gamma = 0.7$ and the finest grid uses $V_\gamma = \frac{0.7}{512}$. The quadtrees used for $V_\gamma = 0.7$, $V_\gamma = \frac{0.7}{2}$, and $V_\gamma = \frac{0.7}{8}$ are presented in Figures 2.5 and 2.6 for mixtures 1 and 2, respectively. Here, the red points are the supporting tie-lines and the green points are the interpolated tie-lines.

Figure 2.7 illustrates typical phase envelopes obtained with CSP interpolation. We can see that phase envelopes are represented by convex piece-wise linear surfaces. Obviously, the smoothness of the surfaces is influenced by the coarseness of the quadtrees.

The interpolation errors obtained with different quadtree resolutions are summarized in Table 2.1. In this example, we sequentially refined the quadtrees by a factor of two starting with the coarsest tree with $V_\gamma = 0.7$. It can be seen that the difference in the $l_2$ norm is insignificant for both mixtures; however, the error is smaller for the mixture 2. This is expected, since we observe an open phase envelop that exhibits weak nonlinear behavior for mixture 2.

### 2.5 Generalized framework based on a multilinear interpolation in tie-line space

The methodology described earlier can be used for the interpolation of the phase compositions, $x_{i,o}$ and $x_{i,g}$. In fact, any function $f = f(\cdot)$ that depends only on tie-line parameters, $\gamma$, and pressure can be interpolated in exactly the same fashion.

The set of unknowns $\{P, L, \gamma\}$ fully parametrizes the sub-critical compositional space; therefore, in the sub-critical region, any property involved in the problem (e.g., phase densities, phase mobilities) is a function of $\{P, L, \gamma\}$ only. Note that the phase compositions depend on the subset of $\{P, L, \gamma\}$, namely, $x_{i,j} = x_{i,j}(P, \gamma)$. Here, we propose a framework that allows for piece-wise linear interpolation with respect to the full set of unknowns, $\{P, L, \gamma\}$. In order to achieve this, the algorithm described
2.5. FRAMEWORK FOR A MULTILINEAR INTERPOLATION

Figure 2.5: Mixture 1: (a) Phase envelope. The discretized tie-line space: (b) $V_\gamma = 0.7$, (c) $V_\gamma = \frac{7}{2}$, (d) $V_\gamma = \frac{7}{8}$
Figure 2.6: Mixture 2: (a) Phase envelope. The discretized tie-line space: (b) $V_\gamma = 0.7$, (c) $V_\gamma = \frac{0.7}{2}$, (d) $V_\gamma = \frac{0.7}{8}$
Figure 2.7: Phase envelopes obtained with CSP interpolation for (left) mixture 1 and (right) mixture 2 columns: (a,d) $V_\gamma = 0.7$, (b,e) $V_\gamma = \frac{0.7}{2}$, and (c,f) $V_\gamma = \frac{0.7}{64}$
Table 2.1: Interpolation error ($l_2$ norm) in phase computations obtained with CSP

<table>
<thead>
<tr>
<th>Refinement</th>
<th>Mixture 1</th>
<th>Mixture 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.8 %</td>
<td>1.14 %</td>
</tr>
<tr>
<td>2</td>
<td>0.87 %</td>
<td>0.82 %</td>
</tr>
<tr>
<td>4</td>
<td>0.49 %</td>
<td>0.35 %</td>
</tr>
<tr>
<td>8</td>
<td>0.22 %</td>
<td>0.043 %</td>
</tr>
<tr>
<td>16</td>
<td>0.09 %</td>
<td>0.01 %</td>
</tr>
<tr>
<td>32</td>
<td>0.04 %</td>
<td>0.0023 %</td>
</tr>
<tr>
<td>64</td>
<td>0.009 %</td>
<td>0.00048 %</td>
</tr>
<tr>
<td>128</td>
<td>0.002 %</td>
<td>0.00012 %</td>
</tr>
<tr>
<td>256</td>
<td>0.0005 %</td>
<td>0.0001 %</td>
</tr>
<tr>
<td>512</td>
<td>0.00013 %</td>
<td>0.0001 %</td>
</tr>
</tbody>
</table>

in Sec. 2.2 was expanded to capture the dependence of the properties on the liquid fraction, $L$. The algorithm for interpolation of an arbitrary function, or property, $X(P, \gamma, L)$ is summarized below:

1. For each pressure in the interval of interest, the tie-line space ($\Gamma$-space) is adaptively constructed in the parameterized domain.

2. Based on the supporting $\gamma$ points, the $\Gamma$-space is tessellated.

3. For any given $\{P, \gamma, L\}$, the function $X(P, \gamma, L)$ is evaluated for the end points of the pressure $[P_j, P_{j+1}]$ and liquid fraction $[L_j, L_{j+1}]$ intervals using interpolation inside the simplex.

4. Bilinear interpolation in the pressure and liquid fraction intervals $P \in [P_j, P_{j+1}]$, $L \in [L_j, L_{j+1}]$ is performed.

Let $\beta(\gamma)^T = [\beta_1(\gamma), \beta_2(\gamma), ... \beta_{n+1}(\gamma)]$ be a vector of barycentric coordinates, $\pi(P)^T = [\pi(P), 1 - \pi(P)]$ is a vector of pressure interpolation coefficients and $\alpha(L)^T = ...$
2.5. FRAMEWORK FOR A MULTILINEAR INTERPOLATION

\[ [\alpha(P), 1 - \alpha(P)] \] is a vector of interpolation coefficients in \( L \). Then, an arbitrary function \( X(P, \gamma, L) \) can be interpolated as follows:

\[
X(P, \gamma, L) = \alpha^T(L) \Pi(P) \ B(\gamma) \ X^*,
\]  

(2.35)

where

\[
B(\gamma) = \begin{vmatrix} \beta^T & 0 \\ 0 & \beta^T \end{vmatrix}, \quad \Pi(P)B(\gamma) = \begin{vmatrix} \pi^T B & 0 \\ 0 & \pi^T B \end{vmatrix}.
\]  

(2.36)

The vector \( X^* \), here, represents the values of \( X(P, \gamma, L) \) evaluated for the end points of the pressure and liquid-fraction interval at the vertices of the simplex. The algorithm is schematically illustrated in Figure 2.8.

Importantly, all interpolation coefficients involved in (2.35) are linear with respect to its unknowns; therefore, Eq. (2.36) defines a multilinear function (product of linear functions).

![Figure 2.8: Interpolation in pressure, liquid fraction and \( \gamma \) parameter](image-url)
2.5.1 Application of the multilinear interpolation framework: synthetic mixing

The EoS accuracy may vary depending on the modeled region of the compositional space and the pressure and temperature ranges (see, for example, Coats (1986)). This lack of accuracy can usually be resolved by component re-lumping or by adjustment of regression parameters for the compositions that lie in the different regions of the compositional space and the $P$-$T$ region.

The generalized CSP framework allows for the use of different EoS types and parameters for different regions along the solution path and, consequently, different regions of the $\Gamma$–space. More importantly, it is possible to replace the EoS model with the phase equilibrium measurements, or one can use a combination of experimental and EoS results. This option may increase the accuracy of the phase equilibrium predictions. Here, we describe one possible application of the complete multilinear interpolation framework. The example presented below is purely synthetic; however, it shows the applicability of the generalized CSP framework to the challenging problem of dynamic component lumping.

For some cases, it may be interesting to lump the hydrocarbon components using different strategies depending on predefined lumping criteria (e.g., based on experimental results or regression analysis). One of the advantages of the CSP approach is the possibility to specify different hydrocarbons mixtures for the different supporting points in the tie-line space. Note that the dimension of the component sets needs to be equal everywhere (i.e., the number of components cannot be changed). This is because the dimension of the tie-line space is fixed. The example below demonstrates the use of two different hydrocarbon mixtures in different regions of the tie-line space. We use the following mixtures: mixture 1 – $\{C_1, CO_2, C_4, C_{10}\}$, and mixture 2 – $\{C_1, CO_2, C_8, C_{10}\}$. The mixtures differ in the intermediate component: $C_4$ is present in the first mixture, and $C_8$ is present in the second.

To demonstrate the power of the CSP approach, we use a simple 1D problem with one injection and one production well. Figure 2.9(a) shows the solution path in tie-line space for both mixtures. Figure 2.9(b) shows the corresponding saturation profiles. It is clear that the solutions for the two mixtures are different. Figure 2.10 shows the solution path and saturation profile for a combined system of mixtures 1
and 2. We use the two mixtures for phase equilibrium computations and properties evaluations at the supporting points for different regions of the tie-line space. The dashed vertical line in Figure 2.10 represents the threshold in the tie-line space that separates regions where different mixtures are used. Figure 2.10 shows that by moving the threshold closer to the injection composition, we can achieve a saturation profile that represents pure mixture 1. A similar strategy may be applied to more realistic problems, where a fluid with a large number of components is lumped differently along the solution path. This strategy, if used carefully, will increase the accuracy of EoS representation.

Figure 2.9: Simulation results for mixtures 1 and 2. (top) Solution paths in the tie-line space, and (bottom) saturation profiles.
2.6 Super-critical space representation

Modeling miscible gas injection processes requires accurate treatment of near- and super-critical regions of the compositional space. However, the super-critical space cannot be parameterized by tie-lines. This is because, by definition, the critical tie-line is the zero-length tie-line, and no tie-lines exist above the critical point. Therefore, the Γ-Variables set cannot be used to represent the super-critical region. However, it is natural to parametrize the space using the pressure and overall compositions, i.e., \{P, z\}, as the set of primary unknowns. Thus, two different sets of unknowns are used to parametrize the entire compositional space: the Γ-Variables and \{P, z\} for the sub- and super-critical spaces, respectively.

Figure 2.11 (a) shows the parameterization used in the Natural Variables formulation. Here, three different sets of unknowns are used, namely: \{P, S_g, x_o, x_g\} for the two-phase region, \{P, x_g\} for the single-phase vapor regions and \{P, x_o\} for the single-phase liquid region. Figure 2.11 (b) presents the parameterization based on the Γ-Variables set; two different sets of unknowns are used for the representation of sub- and super-critical spaces.

As Figure 2.11 (a) indicates, the Natural Variables formulation does not ‘see’ the difference between the super- and sub-critical spaces. This kind of compositional space representation may lead to nonlinear convergence difficulties for miscible gas injection problems (see the Results section). The Γ-Variables formulation, on the other hand, distinguishes between the super- and sub-critical compositions in an effective manner.

Voskov and Tchelepi (2012) showed that on average the Natural Variables formulation provides the best nonlinear convergence for immiscible displacement problems; whereas, the Molar Variables formulation provides better nonlinear behavior for miscible injection. The Γ-Variables set employs a phase-based nonlinear formulation for parameterization of the sub-critical region and a mass-based formulation for super-critical space parametrization. Therefore, the Γ-Variables formulation uses an analog of the Natural Variables formulation for immiscible displacements, and the Molar Variables formulation for modeling miscible problems.

In order to use the Γ-Variables formulation, robust switching criteria between the two sets of unknowns are required. Our algorithm is based on the comparison of the current pressure in the system (gridblock) with the Minimal Critical Pressure (Voskov
Figure 2.10: Simulation results for mixtures 1 and 2. (a) Solution paths in the tie-line space, and (b) saturation profiles for a combined system of mixtures 1 and 2. The dashed vertical lines represent the threshold that separates regions where different mixtures are used.
40

CHAPTER 2. CSP FOR TWO-PHASE DISPLACEMENTS

Figure 2.11: Schematic of the phase diagrams used in the (a) Natural Variables and
(b) Γ-Variables formulation

and Tchelepi, 2008) (MCP) for the given γ. Within the CSP framework, the MCP
can be calculated with arbitrary precision depending on the size of the discretization
simplexes.

Here, we find the MCP for a given value of the γ-parameter using the same inter-
polation technique as described in Section 2.3.1. Namely, the MCP is adaptively
computed and stored at each supporting point. The resulting MCP, which corre-
sponds to the value of a given γ, is found using barycentric interpolation. It is
important to note that the MCP information is crucial for accurate modeling of the
development of miscibility. On the other hand, if the current pressure in the grid cell
is greater than the MCP, a super-critical state is detected and variable substitution
from \{P, L, γ\} to \{P, z\} is performed. For mixtures that form a super-critical fluid,
the procedure described below is performed to obtain the MCP for a given overall
composition, z, and pressure.

If a mixture in a grid cell is parametrized by the \{P, z\} set of unknowns (i.e., the
mixture forms a super-critical fluid), the corresponding MCP must be found. This
can be done in two steps. First, we solve a modified version of (2.4),

\[ z_i - x_{i,o}(P, \gamma)L - x_{i,g}(P, \gamma)(1 - L) = 0, \quad i = 1 \ldots, n_c - 1, \quad (2.37) \]
for the unknown tie-line parameters, $\gamma_i, i = 1..n_c - 2$, and the liquid fraction, for a given $\{P, z\}$. The system of nonlinear equations (2.37) is solved using Newton’s method, where an initial guess is obtained from the previous global Newton iteration for the current timestep. Second, the converged $\gamma$ parameters are used for the computation of the corresponding MCP in order to determine the state of the mixture. Our numerical experiments indicate that the solution of (2.37) is typically obtained within a few nonlinear iterations. If the number of nonlinear iterations exceeds a predefined limit, we assume that the overall composition $z$ is far from the sub-critical boundary (i.e., all supporting points have an MCP lower than the given $P$), and a super-critical state is identified. The main advantages of the proposed variable switching strategy are: (1) continuity of $z$ and $\gamma$ with respect to the change of the mixture state (super- or sub-critical), and (2) local conservation of mass at the global Newton iteration level.

2.7 Simulation Results

Simulation results using our CSP approach are compared with conventional EoS-based computations using the Natural and Molar Variables. We note that the use of the reduced variables (Michelsen, 1986; Hendriks and van Bergen, 1992; Firoozabadi and Pan, 2002; Okuno et al., 2010) or ‘shadow region’ approaches (Rasmussen et al., 2006) reduces the computational time of the thermodynamic related computations significantly. However, these methods were not implemented in the framework used here. Instead, we compared the computational results obtained using the CSP method with another state of the art technique, namely, CSAT (Voskov and Tchelepi, 2009a, 2008). Our extensive numerical experiments show that CSAT provides comparable results to the reduced variables and ‘shadow region’ approaches.

The performance results below indicate that the relative reduction of the computational time achieved with CSP is comparable to that obtained with CSAT. The behavior of the different formulations is compared using four-, five- and eight-component systems. For each of these systems, immiscible and miscible gas displacements are investigated. A brief description of each system is given below.

1. System 1 (four-component system). The initial oil is made up of $\{C_1(20\%)$,
CO\textsubscript{2}(1\%), C\textsubscript{4}(29\%), C\textsubscript{10}(50\%)\} at an initial pressure of 75 bars (above the bubble point). The injection gas is a mixture of two components \{CO\textsubscript{2}(90\%), C\textsubscript{1}(10\%)\}. The production pressure is 50 bars, which is below the bubble-point pressure of the reservoir fluid.

**Immiscible case:** Immiscible gas injection is performed with an injection pressure of 120 bars, which is lower than the Minimum Miscibility Pressure (MMP) for this system.

**Miscible case:** Miscible displacement is performed by increasing the injection pressure to 200 bars, which is higher than the MMP.

For both the miscible and immiscible cases, the difference between the injection and production pressures is quite substantial, which makes the displacement process highly nonlinear because of the changes in the phase state distribution in space and time.

2. System 2 (five-component system). In this system, the initial oil consists of \{C\textsubscript{1}(20\%), CO\textsubscript{2}(1\%), C\textsubscript{4}(19\%), C\textsubscript{8}(40\%), C\textsubscript{15}(20\%)\} at an initial pressure of 75 bars (above the bubble point). The production pressure is 50 bars (below the bubble-point pressure).

**Immiscible case:** The injection gas is a mixture of two components \{CO\textsubscript{2}(80\%), C\textsubscript{1}(20\%)\}. The injection pressure is 120 bars, which is lower than the MMP for the system.

**Miscible case:** The injection composition is a mixture of four components \{C\textsubscript{1}(8\%), CO\textsubscript{2}(80\%), C\textsubscript{4}(10\%), C\textsubscript{15}(2\%)\}; the injection pressure is 200 bars (above MMP).

3. System 3 (eight-component system). The initial oil is a mixture of \{C\textsubscript{1}(10\%), CO\textsubscript{2}(1\%), C\textsubscript{2}(1\%), C\textsubscript{3}(1\%), C\textsubscript{4}(10\%), C\textsubscript{6}(10\%), C\textsubscript{8}(20\%), C\textsubscript{15}(47\%)\} at a pressure of 75 bars (above the bubble point). The production pressure is 50 bars, which is below the bubble-point pressure.

**Immiscible case:** The injection gas is a mixture of two components \{CO\textsubscript{2}(80\%), C\textsubscript{1}(20\%)\}. The injection pressure is 120 bars (below MMP).
Miscible case: The injection composition is a mixture of four components \(\{C_1(10\%), \ CO_2(78\%), \ C_4(10\%), \ C_{15}(2\%)\}\); the injection pressure is 200 bars (above MMP).

All simulations are performed assuming isothermal conditions in the reservoir with a temperature of 373 K.

The porosity and permeability fields are taken from the upper layer of the SPE 10 model (Christie and Blunt, 2001). The size of the model is [60x220x1].

2.7.1 Convergence study

In our approach, only limited numbers of simplexes (and corresponding hyper-cubes) are needed for accurate representation of the thermodynamic phase behavior associated with multicomponent systems. Here, the simulation results obtained with our adaptive parameterization using simplexes of different size are compared with the results of conventional EoS based approaches. In particular, we perform the comparisons for two cases: 1) we only interpolate phase compositions; 2) we do complete interpolations (i.e., phase compositions, densities and mobilities). The size of a simplex is defined as the maximum distance between two supporting points in the simplex, i.e., \(V_\gamma = \|\gamma_i^* - \gamma_j^*\|_\infty\). Since a regular octree is used for the tessellation of the tie-line space, the size of the simplexes does not vary within the tessellation.

Simulation results were performed using a five-component mixture – System 2 (immiscible displacement) and the reservoir model described earlier; the simulation is run for 2000 days.

Figure 2.12 shows three different tessellations used for the convergence study; the sizes of the simplexes vary from very large \((V_\gamma = 0.7)\), Figure 2.12 (a) to relatively small \((V_\gamma = 0.021)\), Figure 2.12 (c). The results obtained with these tessellations and those obtained using the conventional EoS-based method are compared in Figure 2.13. We can see that for the case of interpolation of phase compositions only (Figure 2.13 a,b and c), the largest interpolation error is approximately 20%; whereas, for the case of a refined octree with \(V_\gamma = \frac{0.7}{8}\), the error is insignificant (\(\approx 0.15\%\)). It should be mentioned, however, that the large errors occur mostly around displacement fronts. The same conclusion can be drawn for the case of complete interpolation (Figure 2.13...
c, d and f). The highest error here is substantial (≈ 60%); the error that corresponds to the most refined octree is slightly larger than 1%. The higher error in the case of complete interpolation is caused by significant nonlinearity of the phase mobilities with respect to both \( \gamma \) and liquid fraction. All these observations confirm convergence of the simulation results with tessellation refinement.

It is clear that the size of the simplex, \( V_\gamma \), determines the CSP interpolation error. Therefore, it is important to determine a \( V_\gamma \) that corresponds to the desired interpolation error a-priori. Since the solution path in tie-line space is nearly invariant with respect to changes in the hydrodynamic properties (Entov et al., 2001; Voskov and Tchelepi, 2009a), one can perform fast 1D simulation to assess the interpolation error that corresponds to the chosen \( V_\gamma \). Since the accuracy of the CSP is determined by the nonlinearities of the thermodynamic properties inside the given simplex, the error obtained in 1D may increase during multidimensional simulation, but only slightly.

### 2.7.2 Immiscible gas injection

Immiscible gas injection is modeled for Systems 1-3; in all of these systems, the Minimum Miscibility Pressure is greater than both the injection and initial pressures; hence, the displacement is purely immiscible. In all cases, the simulation was run for 3000 days with \( V_\gamma = 0.176 \). The differences (\( l_2 \) norm) in gas saturation for the different cases are summarized in Table 2.2.

- System 1 (four components): Table 2.2 indicates excellent agreement between the \( \Gamma \)- and conventional EoS-based approaches. The average Courant-Friedrichs-Lewy (CFL) number for this problem is 130, which indicates that the average FIM timestep is 130 times greater than the maximum IMPES timestep. The corresponding tessellated \( \Gamma \)-space is shown in Figure 2.14; it can be observed that small numbers of supporting points and simplexes are sufficient for accurate representation of the dynamics.

Comparison of the performance for different nonlinear formulations is presented in Figure 2.15 (a). It can be seen that the \( \Gamma \)-Variables formulation and the Natural Variables (CSAT) requires the least CPU time. This is attributed to very infrequent stability testing compared with the standard approaches. We
Figure 2.12: Tessellated $\Gamma$-space for the five component system: $V_\gamma = 0.7$ (a), $V_\gamma = 0.176$ (b) and $V_\gamma = 0.021$ (c). Red dots are the supporting tie-lines. Green dots are the interpolated tie-lines.
Figure 2.13: Difference in gas saturation between the $\Gamma$ and Natural variables formulations after 2000 days of simulation: $V_\gamma = 0.7$ (a), $V_\gamma = \frac{0.7}{2}$ (b) and $V_\gamma = \frac{0.7}{8}$ (c)
note that CSAT results in slightly longer stability test times compared with the CSP method. This is due to the displacement character, which occurs mostly around phase boundaries. CSAT requires solution of the full flash system when the feed composition is close to a phase boundary; therefore, the bulk (up to 80\%) of the stability test time is consumed by phase identification for such compositions.

The number of Newton iterations is shown on top of the columns in Figure 2.15. The Natural and Γ-variables formulations show similar numbers of nonlinear iterations; whereas, the Molar Variables simulation needs a greater number of iterations, which leads to the largest CPU time among the three sets.

• System 2 (five components): The simulation results are presented in Figure 2.13 (a) (average CFL ≈ 203). The performance results are shown in Figure 2.16 (a). Here, the Γ-Variables formulation consumes the least CPU time. Again, CSAT requires slightly greater time for stability testing due to the same reasons as in System 1. The Molar Variables formulation shows both the longest simulation time and the largest number of Newton iterations.

• System 3 (eight components): Again, excellent agreement between the Γ- and conventional EoS-based approaches can be observed (Table 2.2). The tessellated Γ-space cannot be shown here, since we deal with a six-dimensional Γ-space; however, we note that only 156 supporting points were used during the simulation. The average CFL number for this problem is 198. The same (as for Systems 1 and 2) conclusions regarding the performance of different nonlinear formulations hold here: the Γ-Variables and Natural Variables (CSAT) formulations incur the least CPU time, and the Molar Variables formulation requires a substantially larger number of Newton iterations (see Figure 2.17 (a)).

2.7.3 Miscible gas injection

Miscible gas injection is modeled using Systems 1-3; in all of these systems, the injection pressure was chosen to be higher than the Minimum Miscibility Pressure in order to achieve miscibility of the injected gas with the initial oil. In all cases the
Figure 2.14: Tessellated Γ-space – System 1.

Figure 2.15: Performance comparison for different nonlinear formulations – System 1. Immiscible (a) and miscible (b) displacements. The number of Newton iterations is shown on top of the columns. The number of wasted iterations is shown in parenthesis.
2.7. SIMULATION RESULTS

Figure 2.16: Performance comparison for different nonlinear formulations – System 2. Immiscible (a) and miscible (b) displacements. The number of Newton iterations is shown on top of the columns. The number of wasted iterations is shown in parenthesis.

Figure 2.17: Performance comparison for different nonlinear formulations – System 3. Immiscible (a) and miscible (b) displacements. The number of Newton iterations is shown on top of the columns. The number of wasted iterations is shown in parenthesis.
Table 2.2: The difference ($l_2$ norm) in gas saturation between the $\Gamma$ and Natural variables formulations

<table>
<thead>
<tr>
<th></th>
<th>Immiscible Injection</th>
<th>Miscible Injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>System 1</td>
<td>0.1 %</td>
<td>2.3 %</td>
</tr>
<tr>
<td>System 2</td>
<td>0.4 %</td>
<td>2.4 %</td>
</tr>
<tr>
<td>System 3</td>
<td>0.2 %</td>
<td>0.6 %</td>
</tr>
</tbody>
</table>

simulation was run for 2000 days with $V_\gamma = 0.176$. The difference ($l_2$ norm) in gas saturation for different cases is summarized in Table 2.2.

- **System 1 (four components)**: Table 2.2 shows good agreement between the $\Gamma$ and Natural variables formulations (the average CFL number is 465).

  As opposed to the immiscible gas injection cases, the Natural Variables formulation shows the greatest number of Newton iterations and the longest CPU time (Figure 2.15 (b)). The $\Gamma$ and Molar variables show similar nonlinear behaviors; however, because of more efficient thermodynamic equilibrium calculations, the $\Gamma$-based approach consumes less CPU time.

- **System 2 (five components)**: Table 2.2 indicates good agreement between the simulations (average CFL $\approx 392$). Similar to the four-component example, the largest interpolation error is observed around miscible fronts.

  The performance results are presented in Figure 2.16 (b). Again, the $\Gamma$-Variables formulation incurs the least CPU time with similar numbers of nonlinear iterations to the Molar Variables formulation. The Natural Variables formulation suffers from a large number of wasted Newton iterations and, consequently, the largest CPU time.

- **System 3 (eight components)**: Figure 2.17 (b) shows the performance results for this problem. These results are in line with those for Systems 1 and 2, and they indicate that the $\Gamma$-Variables enjoys low Newton iterations numbers and the lowest CPU time.
Note that for all three systems, CSAT requires slightly fewer Newton iterations. This is because CSAT employs the SSC approach for identifying the super-critical state instead of the conventional approach based on the component critical temperatures. However, in some cases, CSAT still requires significant time for phase-stability testing.

### 2.7.4 Multiple wells

We compare the CSP simulation results using a more realistic test case. Two five spot patterns are used for the study; the locations and types of the wells are summarized in Table 2.3. For the first 1000 days, the I1 well injects mixture of \{C_1(10\%), \text{CO}_2(80\%), \text{C}_4(10\%\)}; whereas I2 injects \{C_1(70\%), \text{CO}_2(30\%)\}. Both injection wells are operated with constant bottom hole pressure of 120 bars. After 1000 days, both injection wells inject a gas mixture of \{C_1(70\%), \text{CO}_2(30\%)\} at a constant rate of 120000 m$^3$/day. Production wells (P1-P6) are constrained to $P_{bhp} = 30$ bars for the whole simulation run of 1500 days. The initial pressure is set to 85 bars with an initial composition of \{C_1(10\%), \text{CO}_2(1\%), \text{C}_4(9\%), \text{C}_8(40\%), \text{C}_{15}(40\%)\}. Figure 2.18 presents the resulting saturation maps.

The maximum Courant-Friedrichs-Lewy
(CFL) number averaged by the timestep size for this problem is 2500. This indicates that the average FIM timestep is 2500 times greater than the one that an IMPES approach would be able to take. The tessellated Γ-space after 500 (a) and 1500 (b) simulation days is shown in Figure 2.19 where we can clearly see two solution paths corresponding to the two different injection compositions. The $l_2$ differences in gas saturation for the three layers (from top to bottom) are 1.09 %, 1.1 %, and 0.6%.

Figure 2.18: The saturation distribution for three layers after 1500 days of simulation

Figure 2.20 shows a comparison of field oil production and the $l_2$ bottom hole pressure. We can see that the average interpolation error is approximately 1%. Comparison of the performance results for different nonlinear formulations is presented in Figure 2.21. It can be seen that the Γ-Variables formulation and the Natural Variables (CSAT) require the lowest CPU time. This is attributed to less frequent stability testing compared with the standard approaches. Although all three formulations, require approximately the same number of Newton iterations, the Molar Variables formulation consumes significantly more CPU time. We used the overall composition (Voskov and Tchelepi, 2012) based Molar Variables formulation, which requires performing flash computations and implicit derivatives calculations for each
Figure 2.19: Tesselated tie-simplex space after (top) 500 and (bottom) 1500 days of simulation
Newton iteration. Therefore, the properties calculation time is significant for this formulation.

![Figure 2.20: Comparison of field oil rate and bottom hole pressure (I2)](image)

![Figure 2.21: Performance comparison for different nonlinear formulations. The number of Newton iterations is shown on top of the columns.](image)

2.8 Discussion

We presented a general framework of the Compositional Space Parameterization (CSP) method for flow simulation. Here, the governing differential equations are
cast in the compositional tie-simplex, \( \Gamma \)-space. This is possible because a continuous piece-wise linear interpolation in the \( \Gamma \)-space is capable of representing the thermodynamic phase behavior. Analysis of the interpolation error indicates that agreement with reference solutions obtained using standard approaches can be achieved, even when a small number of simplexes is used to discretize the tie-line space. We described a \( \gamma \)-based flash algorithm, that provides a consistent generalization of phase compositions outside the compositional space. We also presented a new and rigorous procedure for identification of the sub- and super-critical regions, developed for simulation of miscible gas injection problems.

The agreement between CSP and conventional methods is quite good, even when a small number of tie-simplexes is used to discretize the tie-simplex space. We showed that the accuracy of complete (multilinear) interpolation can be controlled by refining the tie-simplex space discretization. In terms of computational efficiency, the generalized CSP method reduces the cost of thermodynamic computations significantly and is comparable with CSAT performance. Moreover, we showed that the new tie-line based nonlinear formulation has good convergence behavior for both miscible and immiscible displacements. While further development and testing are needed, the method can be seen as a \( \Gamma \)-Variables formulation for general-purpose compositional simulation.

In our opinion, there are several important aspects of the CSP approach that require additional investigation. These include: investigation of efficient and accurate treatment of near-miscible gas injection; improving the nonlinear solver based on the structure of the solution path in the \( \Gamma \)-space and fractional flow information; developing a sequential-implicit scheme for decoupled multilinear representation of governing equations. Another interesting aspect of compositional simulation that can be studied using the generalized CSP framework is dynamic lumping of components. Although the examples used here are synthetic, they show that the framework allows for the mixing/coupling of different EoS representations based on the solution path characteristics. Therefore, the multilinear framework can serve as a basis for possible dynamic lumping procedures.

One of the possible issues with the CSP framework, which was briefly discussed
in this chapter, is the problem of the existence of solution for the $\gamma$-based flash. Unfortunately, there is no guarantee that a physical solution (phase compositions) of the $\gamma$-based flash exists for the given values of the $\gamma$-parameter, pressure, and temperature. The proposed solution of allowing non-physical phase compositions proved to be effective. However, for some examples, fine discretization of the $\Gamma$-space was needed in order to obtain physical overall compositions after interpolation. Therefore, additional research is needed.
Chapter 3

Three-Phase Thermal Compositional Simulation

3.1 Governing equations

Thermal compositional simulation is widely used to model the behavior of Enhanced Oil Recovery (EOR) processes, such as steam flooding, Steam-Assisted Gravity Drainage (SAGD) (Butler et al., 1981), and Expanding Solvent-SAGD (Nasr and Isaacs, 2001). In thermal compositional simulations, the governing equations that describe the displacement process are the mass (per component) and energy conservation equations. The conservation equations are coupled with the nonlinear thermodynamic relations that describe the instantaneous phase equilibrium of a heterogeneous fluid.

The governing mass conservation equations can be written as:

$$\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{n_p} x_{ij} \rho_k S_j \right) - \text{div} \sum_{j=1}^{n_p} x_{ij} \rho_j u_j + \sum_{j=1}^{n_p} x_{ij} \rho_j q_j = 0, \quad i = 1 \ldots n_c, \quad (3.1)$$

where $i$ indicates a component, and $n_c$ is the total number of components. For a list of symbols, refer to the Nomenclature section.

For thermal simulations, the system of mass conservation equations (3.1) must be solved simultaneously with the energy conservation equation, which can be written
as:

$$\frac{\partial}{\partial t} \left( \phi \left( \sum_{j=1}^{n_p} U_j \rho_j S_j \right) + (1 - \phi) U_R \right) - \text{div} \left( \sum_{j=1}^{n_p} H_j \rho_j u_j \right) - \text{div} (\kappa \nabla T) + \left( \sum_{j=1}^{n_p} H_j \rho_j q_j \right) = 0. \tag{3.2}$$

Similarly to the case of two-phase compositional simulation, additional constraints are needed to close the system of conservation equations (3.1)-(3.2). The first constraints describe the instantaneous thermodynamic phase equilibrium in a gridblock:

$$f_{ij}(P, T, x_{ij}) - f_{ik}(P, T, x_{ik}) = 0, \quad \forall j \neq k = 1 \ldots n_p, i = 1 \ldots n_c. \tag{3.3}$$

Note that the number of phases, $n_p$, is equal to three; the phases are: 1) water, 2) oil, and 3) vapor.

The system is supplemented with linear constraints for the component phase compositions and phase saturations, namely,

$$\sum_{i=1}^{n_c} x_{ij} = 1, \quad j = 1 \ldots n_p, \tag{3.4}$$

$$\sum_{j=1}^{n_p} S_j = 1. \tag{3.5}$$

Eqs. (3.1)-(3.5) describe the multiphase thermal-compositional problem.

One of the challenges associated with compositional simulation is accurate identification of the phase state of the mixture in a given gridblock. For two-phase systems that involve vapor (gas) and liquid (oil) phases, there are three possible combinations of the phase state: 1) single-phase gas, 2) single-phase oil, and 3) a two-phase state. However, for mixtures that can form three phases, the number of possible combinations is seven, namely, three single phase states, three combinations of two-phase mixtures, and a three-phase state.

During three-phase simulations, the phase-behavior of the fluid mixture is usually described by using K-value tables (Coats, 1980a; Aziz and Wong, 1989). The approach based on the predefined K-value tables is commonly referred to as the K-values method. The K-values method for isothermal compositional simulation, for
example, uses a predefined table where the K-values are only represented as a function of pressure. This method is known to be adequate for oil recovery problems where the K-values are weak functions of composition. Several methods for accuracy improvement of the K-values representation in the case of two-phase compositional simulation have been proposed (Young and Stephensen, 1983; Rannou et al., 2013). In the case of thermal simulation, the K-values table depends on both pressure and temperature. In addition, since hydrocarbon components can dissolve in the water phase, liquid-liquid interactions are sometimes included in the K-value tables. The K-values based method is implemented in virtually all industrial thermal reservoir simulators (CMG STARS, 2009; Schlumberger Eclipse, 2000).

Although computationally attractive, the K-values approach can lead to significant errors in the phase-behavior representation, especially for near-miscible displacements. On the other hand, the EoS-based approach can be more accurate, but significantly less efficient (Aziz and Wong, 1989). The main difficulty of EoS-based computations lies in the complexity of the thermodynamic expressions that describe general multicomponent systems, as well as the iterative nature of the solution method. This complexity grows substantially with the number of phases and components. The use of EoS-based phase-behavior computations for three-phase thermal simulation has been investigated by Varavei and Sepehrnoori (2009); Iranshahr (2012); Heidari (2014); Zaydullin et al. (2014b).

3.1.1 Phase Equilibrium Computations

In this section, we describe the phase-equilibrium computations that are necessary for the K-values- and EoS-based approaches. For the EoS-based approach, the phase-behavior computations are similar to those employed in two-phase compositional simulation. Namely, a combination of stability testing (Michelsen, 982a) and flash computations is used to determine the phase state and phase compositions for a given pressure, temperature, and composition. However, here the number of phase stability tests required is higher due to the larger number of possible phase combinations. When a new phase appears, multiphase flash calculations are typically performed to obtain phase compositions for the new phase(s). The correct solution of the multiphase flash should satisfy the global minimum of the Gibbs-free energy, but finding
this global minimum usually requires a significant computational effort (compared to the case of two-phase systems). In our work, we use two multiphase EoS-based libraries described by Lucia and Feng (2003) and by Petitfrere and Nichita (2014).

In case of the K-values method, the phase stability test algorithm can be simplified significantly; the simplification is due to the assumption of compositional independence of the K-value tables. Indeed, a phase composition \( \mathbf{x} \) is stable at a given pressure and temperature, if the following condition is satisfied (Michelsen, 82a):

\[
1 + \sum_{i=1}^{n_c} Y_i (\ln Y_i + \ln \phi_i(Y) - \ln(x_i) - \ln \phi_i(x) - 1) \geq 1, \quad (3.6)
\]

where \( y_i \) denotes a trial composition, \( \phi_i() \) is the fugacity coefficient of component \( i \), and \( Y_i \) is a mole number. Now, because the K-values are independent of the phase compositions \( \mathbf{x} \) and \( \mathbf{y} \), we can write that:

\[
Y_i = K_i x_i, \quad i = 1 \ldots n_c, \quad (3.7)
\]
\[
\phi_i(y) = \frac{\phi_i(x)}{K_i}, \quad (3.8)
\]
\[
\phi_i(Y) = \phi_i(y). \quad (3.9)
\]

Substituting trial phase compositions and fugacity coefficients in Eq. (3.6) using relationships (3.8 - 3.9), we obtain that the phase associated with composition \( \mathbf{x} \) is stable if and only if:

\[
\sum_{i=1}^{n_c} K_i x_i \leq 1. \quad (3.10)
\]

It is evident from Eq. (3.10) that phase stability testing for the K-values method does not require any iteration. As a result, phase stability testing for the K-values method is typically an order of magnitude faster when compared to the EoS-based approach (see, for example, Rannou et al. (2013)).

The flash calculations for the K-values method reduces to the solution of a generalized Rachford-Rice equation (Iranshahr, 2012). Also, the fugacities in Eq. (3.3)
are replaced with the corresponding K-values constraints:

\[ x_{i,o} - K_{i,go}^{-1} x_{i,g} = 0 \quad i = 1 \ldots n_c, \]  
\[ x_{i,o} - K_{i,wo}^{-1} x_{i,w} = 0 \quad i = 1 \ldots n_c, \]

where \( x_{i,j} \) is the phase composition of component \( i \) in phase \( j \in \{o, w, g\} \), \( K_{i,go} \) is the K-value of component \( i \) that defines oil-gas interaction, and \( K_{i,wo} \) is the K-value of component \( i \) that determines oil-water interaction.

### 3.1.2 Comparison with CMG-STARS

Results for simulations using AD-GPRS are compared with results using the commercial reservoir simulator, CMG-STARS (CMG STARS, 2009). For the purpose of this comparison, we model the SAGD process for a single well pair. The following is a list of input parameters:

- Three-component fluid \( \{CO_2(1\%), Bitumen(27\%), H_2O(72\%)\} \); initial oil saturation of 0.8.
- Reservoir grid containing 25 x 1 x 25 cells,
- Physical dimensions of \([50 \times 800 \times 25]\) m³,
- Uniform permeability of 2000 mD and constant porosity of 0.32,
- Distance of 5m between the injection (upper) and production (lower) wells,
- Initial pressure of 8.1 bar at the top of reservoir
- Uniform initial temperature of 290 K,
- Injection of superheated steam at 25 bar.

One difference between the AD-GPRS and CMG-STARS simulators is the manner of performing the phase-behavior computations. In CMG-STARS, the phase-behavior can only be described using pre-defined K-value tables, which are pressure-temperature (P-T) dependent. As previously discussed, AD-GPRS supports the EoS
and K-value-based methods. Therefore, in order to validate the simulation results in this work, P-T dependent K-values tables are generated using the AD-GPRS internal EoS-based algorithm. These tables are then used for CMG-STARS and AD-GPRS simulation runs. In addition, all properties in AD-GPRS are adjusted to support the CMG-STARS correlations. Specifically,

- Phase densities are modeled using the *MOLDEN keyword (includes compressibility).
- Phase enthalpies are modeled using the *CPG and *HVAP correlations.
- Phase viscosities are modeled using the *VISCTABLE keyword.

Figures 3.1 and 3.2 show the oil and gas saturation distributions and temperature profiles after 450 and 810 days of simulation, respectively. The agreement between the two simulators is quite good; the small mismatch can be attributed to the use of slightly different time-stepping strategies and different convergence tolerances. Figure 3.3 depicts the cumulative steam-to-oil ratios for AD-GPRS and CMG-STARS. Again, a very close match is observed for the two simulators.

This simple validation study confirms that AD-GPRS is capable of reproducing the results of a commercial simulator when the physics of the displacement process is described using a simplified phase-behavior model (i.e., K-value tables).

### 3.2 Comparison of EoS-based and K-value methods

In this section, we study the impact of the simplification assumption (compositional independence) used in the K-values method. In order to make a consistent comparison, the K-value tables are generated using a three-phase EoS-based K-value generator. In other words, we compare simulation results obtained using the EoS-based phase equilibrium model with those obtained with the K-values method, where the K-values are generated using the same EoS model. Also, since the three-phase EoS model allows for solubility of all components in any phase (e.g., the water component can dissolve in the oil phase), the liquid-liquid interactions are included in the
3.2. COMPARISON OF EOS-BASED AND K-VALUE METHODS

Figure 3.1: Simulation Results After 450 Days: CMG-STARS (left) and AD-GPRS (right)

Figure 3.2: Simulation Results After 810 Days: CMG-STARS (left) and AD-GPRS (right)
generated K-value tables.

A very simple reservoir model is used here. The reservoir is comprised of [3000x1x1] gridblocks and the total reservoir volume of [200x1x1] m$^3$. The other reservoir parameters are:

- Uniform initial pressure and temperature of 25 bar and 370 K.
- Dirichlet boundary conditions: pressure at the left corner of 27 bar (fixed temperature of 505 K); pressure at the right corner of 20 bar (fixed temperature of 370 K).
- Uniform permeability of 4000 mD and a constant porosity of 0.3.
- Rock thermal conductivity of 1.86x10$^2$ KJ/m-day-K.

For the first set of simulations, a four-component fluid is used; the components are $\{C_1(0.1\%), iC_4(1\%), Bitumen(24.9\%), H_2O(74\%)\}$. The component parameters are listed in Table 3.1. At the initial pressure and temperature, the fluid forms an oil-water mixture with an oil saturation of 0.8012. Using this fluid, we perform a series of simulations that differ only in the type of the injected fluid:
1. Injection of pure steam,

2. Injection of steam and non-condensable solvent, \{C_1(30\%), H_2O(70\%)\},

3. Injection of steam and condensable solvent, \{C_1(5\%), iC_4(25\%), H_2O(70\%)\}.

Table 3.1: Thermodynamic Properties for \{C_1, iC_4, Bitumen, H_2O\} fluid

<table>
<thead>
<tr>
<th>Component</th>
<th>T_c K</th>
<th>P_c bar</th>
<th>\omega</th>
<th>M_w g/mol</th>
<th>k_{i,C_1}</th>
<th>k_{i,Bitumen}</th>
<th>k_{i,H_2O}</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_1</td>
<td>190.56</td>
<td>46.04</td>
<td>0.013</td>
<td>16.04</td>
<td>0</td>
<td>0.081</td>
<td>0</td>
</tr>
<tr>
<td>iC_4</td>
<td>425.2</td>
<td>37.96</td>
<td>0.201</td>
<td>58.12</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Bitumen</td>
<td>819.307</td>
<td>34.56</td>
<td>0.516</td>
<td>72.15</td>
<td>0.081</td>
<td>0</td>
<td>0.1658</td>
</tr>
<tr>
<td>H_2O</td>
<td>647.37</td>
<td>221.2</td>
<td>0.345</td>
<td>18.015</td>
<td>0</td>
<td>0.1658</td>
<td>0</td>
</tr>
</tbody>
</table>

Simulations are performed using both the K-values and EoS-based methods. For these comparisons, we used K-values that were tabulated using very fine discretization in pressure and temperature. Namely, we constructed the K-value tables using pressure increments of 0.5 bar, and temperature increments of 3.2 K. Importantly, all of the phase properties (i.e., densities, viscosities, enthalpies) are computed using correlations that are exactly the same for both approaches. Moreover, the viscosities for C_1 and iC_4 are assumed to be identical. The identical viscosities of C_1 and iC_4 is not a limitation of our simulator. The assumption is made in order to focus on the impact of the thermodynamic behavior only. Also, in order to minimize the time-truncation error, a small maximum timestep of 0.1 days (CFL < 1) was used. A tight tolerance of 1E-6 was used to ensure convergence of the material balance. This set-up allows for consistent comparison of the K-values and EoS-based methods (where the only difference is in the phase-behavior computations).

Simulation results for the case of pure steam injection are shown in Figure 3.4, which plots the gas saturation and the overall composition profiles at 2500 days. The mismatch in the profiles between the two methods is located mainly at the edge of the iC_4 bank. This bank forms due to condensation of iC_4, which moves ahead of
the temperature front. Since the injection fluid does not contain any $iC_4$ component, the bank is composed of the original $iC_4$ present in the reservoir. It is obvious that this bank could be more pronounced, if a larger amount of $iC_4$ was present in the reservoir.

Figure 3.5 presents compositional diagrams for both methods obtained after 2500 days. The black point denotes the initial composition, the yellow point denotes the injection composition, and the green points represent the solution path. Here, we can observe that part of the compositional profile lies in the area where the amount of $iC_4$ is larger than the injection, or initial, amounts. The red triangles in the compositional space represent tie-simplexes that are built for the compositions around the $iC_4$ bank. A clear difference between the tie-simplexes obtained with the K-values and EoS methods can be observed in the area closer to the \{$C_4$,Bitumen, $H_2O$\} face of the compositional space. This area corresponds to the part of the displacement profile that has a larger amount of the $iC_4$ component. The two tie-simplexes are different due to the assumption of compositional independence of the K-value tables, which translates into linear phase-envelope boundaries. The fact that part of the compositional profile lies in the area where the K-values-based phase-envelope differs from the one based on the EoS representation indicates that the displacement is near-miscible. It is known that the use of the K-values method leads to larger errors in phase-equilibrium representation for near-miscible displacements, and we can clearly observe these errors in the displacements profiles in Fig. 3.4.

The next simulation involves injection of steam and non-condensable solvent, \{$C_1(30\%), H_2O(70\%)$\}. Figure 3.6 shows the simulation results for both methods at 2500 days, and a perfect match between the two methods can be observed. Note that the $iC_4$ bank does not form in this case due to the presence of a large amount of non-condensable gas in the system. The compositional spaces are presented in Figure 3.7; the color-code in the figure is the same as in Fig. 3.5. Note that the solution structure for these types of displacements in the isothermal case has been thoroughly discussed in LaForce et al. (2008b,a, 2009). Since, for this example, a $iC_4$ bank does not form, the displacement occurs predominantly in the \{$C_1$, Bitumen, $H_2O$\} ternary plane. We can observe a shock directly from the \{$C_1$, $H_2O$\} injection mixture into
Figure 3.4: Displacement profiles for \( \{C_1, iC_4, Bitumen, H_2O\} \) fluid: pure steam injection
Figure 3.5: Compositional Space for pure steam injection case at $T = 400 \text{ K}$ and $P = 26.8 \text{ bar}$: (a) EoS-based simulation (b) K-values-based simulation. The green points are the solution path, the black point is initial oil and the yellow point is injected gas.
the three-phase region of \( \{ C_1, \text{Bitumen}, H_2O \} \) followed by a long rarefaction, another shock to the \( \{ \text{Bitumen}, H_2O \} \) binary, and finally a rarefaction to the initial composition. Since the displacement occurs primarily in the \( \{ C_1, \text{Bitumen}, H_2O \} \) plane, the tie-simplexes involved in the displacement process lie in the same plane and differ only due to the pressure and temperature variation. Figure 3.7 shows two of these tie-simplexes evaluated at the \( T = 370K \) (red) and \( T = 480K \) (blue). We can see that these tie-simplexes are very similar for the K-values and EoS methods.

Finally, we perform a simulation where steam is coinjected with a condensable solvent. The simulation results are shown in Figure 3.8. Figure 3.8 shows the gas saturation and overall composition profiles at 2500 days. The difference in the results obtained with the two methods is substantial. We can clearly observe significant differences between the profiles near the bank of the injected \( iC_4 \). This bank is much larger compared with the one obtained in the pure steam injection case. The structure of the displacement is shown in Figure 3.9. Similar to the \( \{ C_1, H_2O \} \) injection case, we can see a shock from the injection composition to the three-phase region; however, since a mixture of \( \{ C_1, C_4, H_2O \} \) is injected, the shock now lands in the region where all components exist. The shock is followed by a rarefaction within a three-phase region; this rarefaction is then followed by a shock, and a spreading wave that lands at the water corner. From the water corner, we can observe a series of shocks and rarefactions to the initial composition. The tie-simplexes depicted in Figure 3.9 are built in the area where significant amounts of \( iC_4 \) are present (a long spreading wave in Fig. 3.8). We can observe that the tie-simplexes are tilted in the case of the EoS-based simulation. As in the case of pure steam injection, the difference of the phase-envelopes boundaries corresponds to the area of higher \( iC_4 \) concentration. However, in this case, since \( iC_4 \) is injected, a large portion of the compositional profile lies in the area where the phase envelopes are different for the two methods. The difference in the phase-envelope representation in this region leads to a large mismatch in the displacement profiles in Figure 3.8.

For the second set of simulation runs, we employ the same 1D reservoir description used previously; however, a different fluid system is used. We replace the \( iC_4 \) component with the lighter \( C_3 \) component. Now, the initial oil-water mixture is formed by \( \{ C_1(0.1\%), C_3(1\%), \text{Bitumen}(24.9\%), H_2O(74\%) \} \). Evaluation of all properties
Figure 3.6: Displacement profiles for \(\{C_1, iC_4, \text{Bitumen}, H_2O\}\) fluid: steam and non-condensable solvent injection.
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Figure 3.7: Compositional Space for steam and non-condensable solvent injection case: (a) EoS-based simulation (b) K-values-based simulation. The green points indicate the solution path, the black point marks the initial oil composition and the yellow point marks the injected gas composition.

remains the same as for the heavier component example. Importantly, the viscosities of the components are assumed to be identical to the corresponding viscosities used in the previous runs. Therefore, the only difference between the two sets of simulations (using different fluids) is in the phase-equilibrium computations for the different fluids. The initial pressure and temperature remain the same as in the previous simulation; the oil and water saturations at reservoir conditions are 0.8011 and 0.1989, respectively. Using this fluid, we perform two sets of simulations that differ only in the type of injected fluid:

1. Injection of steam and non-condensable solvent, \(\{C_1(30\%), H_2O(70\%)\}\),

2. Injection of steam and condensable solvent, \(\{C_1(5\%), iC_3(25\%), H_2O(70\%)\}\).

Simulation runs are performed using the K-values and EoS-based methods. As in the previous case, all of the phase properties (i.e., densities, viscosities, enthalpies) are computed using correlations that are exactly the same for both approaches.

The first simulation is the coinjection of steam and non-condensable solvent (methane). The displacement profiles obtained at 1800 days are presented in Figure 3.10. Similar
CHAPTER 3. THREE-PHASE THERMAL COMPOSITIONAL SIMULATION

Figure 3.8: Displacement profiles for \( \{C_1, iC_4, Bitumen, H_2O\} \) fluid: steam and condensable solvent injection
Figure 3.9: Compositional Space for steam and condensable solvent injection case at $T = 400$ K and $P = 26.8$ bar: (a) EoS-based simulation (b) K-values-based simulation. The green points indicate the solution path, the black point marks the initial oil composition and the yellow point marks the injected gas composition.
to the case where a heavier intermediate component \(iC_4\) is injected, we can observe a perfect match between the K-values and the EoS-based simulations. The solution structure in the compositional space is demonstrated in Figure 3.11. The structure of the solution is exactly the same as in the case of the steam and non-condensable solvent injection using the \(iC_4\) component. The two tie-simplexes depicted in Figure 3.11 are evaluated at the temperatures of 370 K (red) and 480 K (blue). We can see the two methods result in nearly identical tie-simplexes. Therefore, since the phase-behavior representation is quite similar for the two methods, we can observe almost identical saturation and composition profiles in Figure 3.10.

Similar to the previous examples, we perform a simulation where a \(\{C_3(25\%) - C_1(5\%)\}\) mixture is coinjected along with the steam. The gas saturation, water, bitumen, and propane overall compositions after 1800 days are presented in Figure 3.12. Here, we can observe a bank of the \(C_3\) component that moves slightly faster relative to the steam front. Also, we can see that the results from the K-values method deviate from those obtained using EoS mainly around the \(C_3\) bank location. This observation is consistent with the previous simulation when the \(\{iC_4(25\%) - C_1(5\%)\}\) mixture was injected. However, in this case the differences are significantly smaller. The solution structures for both methods are shown in Figure 3.13. They are similar to the ones obtained with the injection of \(iC_4\) as a solvent. The tie-simplexes shown in Figure 3.13 are built in the area of increasing amounts of \(C_3\). In contrast to the \(iC_4\) injection case, the tie-simplexes are quite similar. We can see that the phase-envelopes are nearly linear for both cases (tie-simplexes are not tilted). The similarity of the tie-simplexes is due to the immiscible conditions of the displacement for the case of \(C_3\) injection compared with the previous runs, where a heavier solvent was injected. Due to the similar phase-behaviors, the profiles in Figure 3.12 do not differ substantially.

### 3.2.1 3D Steam-Solvent Coinjection

The next set of simulations deals with steam-solvent coinjection in a three-dimensional, layer-cake reservoir. The model is comprised of \([40\times40\times6]\) gridblocks; where the first two layers represent the under- and over-burdens. The total reservoir volume (four layers) is \([1200\times1200\times2.5]\) m\(^3\). The other reservoir parameters are:
Figure 3.10: Displacement profiles for \{C_1, iC_3, Bitumen, H_2O\} fluid: steam and non-condensable solvent injection
CHAPTER 3. THREE-PHASE THERMAL COMPOSITIONAL SIMULATION

Figure 3.11: Compositional Space for steam and non-condensable solvent injection case: (a) EoS-based simulation (b) K-values-based simulation. The green points indicate the solution path, the black point marks the initial oil composition and the yellow point marks the injected gas composition

- Uniform initial pressure and temperature of 20 bar and 350 K.
- Constant porosity of 0.33.
- Layer horizontal permeabilities are $[2500, 2000, 1000, 500]$ md.
- Layer vertical permeabilities are $[250, 200, 100, 50]$ md.
- Rock thermal conductivity of $1.86 \times 10^2$ KJ/m-day-K.

The fluid description is the same as in the 1D examples above where $iC_4$ was used as an intermediate component. The resident fluid is composed of $\{C_1(0.1\%), \ iC_4(2\%), \ Bitumen(23.9\%), \ H_2O(74\%)\}$ with uniform initial temperature of 350 K and pressure of 20 bar. The initial oil and water saturations are 0.798 and 0.202, respectively. A single injection well is placed in the center of the reservoir; six wells are used to produce the resident oil.

We perform two sets of simulation runs to compare the K-values and EoS-based methods. The first set of simulations involves the injection of steam and solvent with
Figure 3.12: Displacement profiles for \{C_1, iC_3, Bitumen, H_2O\} fluid: steam and condensable solvent injection
Figure 3.13: Compositional Space for steam and condensable solvent injection case at $T = 400$ K and $P = 26.8$ bar: (a) EoS-based simulation (b) K-values-based simulation. The green points indicate the solution path, the black point marks the initial oil composition and the yellow point marks the injected gas composition.
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a high concentration of $iC_4$ in the injection stream. The injection composition here is \{C_1(4\%), iC_4(12\%), H_2O(84\%)\}. For the second set of simulations, we reverse the C_1 and iC_4 concentrations; that is, we inject a mixture of \{C_1(12\%), iC_4(4\%), H_2O(84\%)\}. For both sets of simulations, we compare the K-values and EoS-based methods. The injection and production conditions are the same for all simulations: the injector is operated at a constant bottom-hole pressure (BHP) of 50 bar with steam quality of 0.8 and steam pressure of 40 bar; all production wells are set at a constant BHP of 3.5 bar. The rates are reported at the reservoir conditions.

Figure 3.14 shows the oil saturation, gas saturation, and temperature maps, for the case of \{C_1(4\%), iC_4(12\%), H_2O(84\%)\} injection, after 3000 days; here the EoS-based phase representation is used. The results are presented for the four layers, excluding the under and over burdens. In addition, Figure 3.15 shows the difference maps for the K-values and EoS-based simulations. The maps are constructed by subtraction of the saturation and temperature values obtained with the K-values method from the corresponding values obtained with the EoS-based method. Figure 3.16 shows field cumulative oil rates (at reservoir conditions) for the two methods. As illustrated in both figures, the difference in the simulation results of two methods is significant. These results confirm that our observations for the 1D simulations are reproducible for a more realistic 3D model.

The simulation results for the second set of simulations are demonstrated in Figures 3.17, 3.18, and 3.19. Here, we can observe that the mismatch between the simulation results for the two methods is less significant. We note that this observation is consistent with the simple 1D simulations reported earlier in this chapter.

3.2.2 ES-SAGD simulation

The last set of simulations compares the K-values and EoS-based approaches for the modeling of the ES-SAGD process (Nasr and Isaacs, 2001). Here, we use a 2D reservoir with a pair of horizontal wells. The reservoir consists of [100x1x50] gridblocks with spatial dimensions of [50x800x25] m^3. The reservoir is preheated for 120 days with hot water injection. We use the two fluids previously presented for the comparison of the two methods. The initial pressure and temperature distributions are the same for both cases: constant temperature of 290 K and a pressure of 18.2 bar at the
Figure 3.14: 3D example with \( \{C_1(4\%), \ iC_4(12\%), \ H_2O(84\%)\} \) injection: saturation and temperature maps obtained using the EoS-based approach for four layers.
Figure 3.15: 3D example with \(\{C_1(4\%), \ iC_4(12\%), \ H_2O(84\%)\}\) injection: difference maps between EoS- and K-values-based approaches for four layers
Figure 3.16: 3D example with \{C_1(4\%), iC_4(12\%), H_2O(84\%)\} injection: field cumulative oil rates

top of the reservoir. The initial component distributions are identical to the 1D simulations. The injected fluids are \{C_3(10\%), H_2O(90\%)\} and \{iC_4(10\%), H_2O(90\%)\} for the cases of using C_3 and iC_4 as an intermediate component, respectively.

Figure 3.20 (a) presents the oil saturation, gas saturation, and temperature maps after 500 days of simulation obtained using the \{C_1, C_3, Bitumen, H_2O\} fluid mixture. Figure 3.20 (b) shows the difference maps for this simulation. We can observe that the saturation maps differ mainly around the gas saturation front where the amount of injected solvent is high. However, this difference disappears as soon as the steam front reaches the area of high solvent concentration (the solvent propagates ahead of the steam front). This observation is confirmed by the plot of cumulative oil production (Figure 3.21), where we can see that the difference in terms of oil production rates is insignificant.

Next, a simulation example of ES-SAGD is performed with injection of \{iC_4(10\%), H_2O(90\%)\}. For this example, the saturation and temperature maps are demonstrated in Figure 3.22 (a). The difference maps are shown in Figure 3.22 (b). As
3.2. **COMPARISON OF EOS-BASED AND K-VALUE METHODS**

Figure 3.17: 3D example with $\{C_1(12\%), iC_4(4\%), H_2O(84\%)\}$ injection: saturation and temperature maps obtained using the EoS-based approach for four layers.
Figure 3.18: 3D example with \{C_1(12\%), \, iC_4(4\%), \, H_2O(84\%)\} injection: difference maps between EoS- and K-values-based approaches for four layers.
3.3 Discussion

We presented two methods for phase-equilibrium computations for three-phase thermal simulation. We showed that the commonly used K-values method does not require any iteration for phase-stability testing; therefore, it can be an order of magnitude faster than EoS-based simulation. In fact, for the ES-SAGD examples, the EoS-based phase appearance computations are on average 20 times slower than those of the K-values method.

We showed that the difference in simulation results for the two methods can vary from negligible to substantial depending on the details of the displacement process.

Figure 3.19: 3D example with \( \{C_1(12\%), \ iC_4(4\%), \ H_2O(84\%)\} \) injection: field cumulative oil rates

in the previous example, we can see that 1) the deviation from the EoS-based results occurs mostly at the solvent front, and 2) the cumulative oil rates (Figure 3.23) obtained using the two methods are similar.
Figure 3.20: ES-SAGD Example with \{C_1, C_3, Bitumen, H_2O\}: oil saturation, gas saturation, and temperature maps obtained with EoS-based approach (left); saturation and temperature difference maps (right)
3.3. DISCUSSION

Figure 3.21: ES-SAGD Example with \{C_1, C_3, Bitumen, H_2O\}: cumulative oil production rate
Figure 3.22: ES-SAGD Example with \{C_1, iC_4, Bitumen, H_2O\}: oil saturation, gas saturation, and temperature maps obtained with EoS-based approach (left); saturation and temperature difference maps (right)
3.3. DISCUSSION

Figure 3.23: ES-SAGD Example with \{C_1, iC_4, Bitumen, H_2O\}: cumulative oil production rate
The 1D simulation examples helped to explain the simulation results. We demonstrated that the use of heavier solvents can lead to significant differences in the phase-behavior representation when the phase-envelope becomes nonlinear. For such cases, the simulation results for the two methods differ significantly. On the other hand, the case of the injection steam and non-condensable solvent showed that the K-values method can adequately model displacements that are far from miscibility conditions. However, a steam injection case showed that even in the absence of any solvent, the simulation results from the two methods can differ, if there is an accumulation (bank) of condensable gas.

Finally, ES-SAGD examples revealed that the mismatch between the simulation results obtained with the K-values and EoS methods not only depends on the type of solvent and (P-T) conditions, but also on the recovery process. In the case of ES-SAGD (and SAGD), the recovery primarily occurs due to the interplay between gravitational force and the temperature induced viscosity reduction of the resident oil. Therefore, in the case of very heavy oil (Bitumen), accurate phase-behavior representation may not be important.

We note that comparisons of the K-values and EoS-based simulation results for ES-SAGD processes have been reported in Varavei and Sepehrnoori (2009); Heidari (2014). However, we think that those studies did not provide a clear explanation of the differences observed for the two methods. For example in Varavei and Sepehrnoori (2009), the difference in the simulation results were attributed to the solubility of water in the oil phase and the solubility of hydrocarbons in the water phase, since the liquid-liquid interactions were not modeled using K-values. The comparison in Heidari (2014) were performed using ES-SAGD examples, where the phase-behavior effects are hard to isolate from the other complex displacement mechanisms. Our 1D simulation study, however, demonstrated that the mismatch in the results is clearly due to the development of miscibility for the cases where significant concentrations of the intermediate component are present in the reservoir.
Chapter 4

Bypassing Strategies for Phase-State Identification

In the previous chapter we showed that representation of the thermodynamics associated with three-phase thermal-compositional processes may require full EOS calculations. Using a three-phase EoS model is necessary for modeling processes that involve injection of both steam and solvent, as well as displacements that involve the development of misciblity between the resident oil and the injected fluid. Another example for which three-phase EoS modeling may be needed is low-temperature (below 320K) CO$_2$ injection for which three hydrocarbon phases can form. These phases are a CO$_2$-rich liquid phase, an oil phase, and a vapor phase. In our experience, for low-temperature CO$_2$ injection problems, use of a conventional two-phase compositional description can result in significant convergence problems. These convergence issues are clearly attributable to the use of two-phase stability and flash calculations, which lead to arbitrary/wrong labeling of the liquid phases. Moreover, for this class of problems, where three-phase compositional effects important, the standard K-values method is not viable. Therefore, three-phase EoS phase equilibrium representation is necessary for adequate modeling of such displacement processes.

Accurate representation of thermodynamic equilibrium for three-phase systems is considerably more expensive than for two-phase mixtures. This is mainly because of the large number of phase-state combinations (seven combinations), which can exist for a given multicomponent system.
Several methods have been proposed to speed-up the EoS-based computations for two-phase compositional problems. One very powerful approach is the ‘shadow region’ method (Rasmussen et al., 2006) for bypassing the phase-stability test using information about the compositional space in the neighborhood of the subject composition. This method has proved to be efficient for two-phase compositional simulation. However, the ‘shadow region’ method has not been generalized to the cases of three- (or more) phases.

Other methods were developed that make use of findings from gas-injection theory (Dindoruk et al., 1997; Orr et al., 1993; Orr, 2007) have been developed. The general framework that extends the theory to numerical, multi-dimensional compositional simulation is described in Chapter 2 and is referred to as Compositional Space Parametrization (CSP). A related technique is the Compositional Space Adaptive Tabulation (CSAT) for bypassing phase-stability testing (Voskov and Tchelepi, 2009a, 2008). The two-phase CSAT method can be viewed as a specific realization of the general CSP framework.

The CSAT approach was later extended to handle three-phase systems, where tie-triangles and their extensions are adaptively constructed, collected, and parameterized (Iranshahr et al., 2013). However, while the extended CSAT approach is efficient, it relies on having detailed geometrical properties of the compositional space, especially of the two-phase regions that surround the tie-triangles.

Here, we extend the CSP framework by introducing a method for bypassing the phase identification computations for multicomponent systems that can form three, or more, phases. The method is aimed at minimizing the number of multiphase flash calls during a flow simulation. Several examples are presented, including three-phase steam-solvent injection, and cold CO$_2$ injection. The method has been summarized in Zaydullin et al. (2014a).

4.1 Phase Identification based on CSAT

In this section, we summarize the previously developed CSAT method. More information and numerical results can be found in Iranshahr et al. (2013).
Three-phase Negative-Flash

One of the key components of the CSP family of methods is a generalized multiphase negative-flash method (Iranshahr et al., 2010). In the negative-flash method, one solves the system of Eq. (3.3) along with the following constraints:

\[ z_i - \sum_{j=1}^{n_p} x_{ij} \nu_j = 0, \quad i = 1 \ldots n_c, \quad (4.1) \]

\[ \sum_{i=1}^{n_c} (x_{i1} - x_{ij}) = 0, \quad j = 2 \ldots n_p. \quad (4.2) \]

For a pre-assumed maximum number of phases, \( n_p^{\text{max}} \), the combination of Successive Substitution Iterations (SSI) and a damped Newton method can be used to solve the problem in a manner similar to that used for a standard flash. However, unlike the standard flash procedure, the phase fractions, \( \nu_j \), are not limited to the physical interval \((0, 1)\).

The advantage of this approach is that if all \( n_p^{\text{max}} \)-phases exist at the given conditions \( (P \text{ and } T) \), the negative-flash will converge to a unique solution (Iranshahr et al., 2010). If the solution belongs to a tie-simplex \( \Delta \), which is defined as:

\[ \Delta = \{ \nu \in \mathbb{R}^{n_p-1} \mid 0 \leq \nu_j \leq 1, \forall j \}, \quad (4.3) \]

and the number of phase \( n_p = n_p^{\text{max}} \), then this solution satisfies the global minimum of the Gibbs-free energy. If the solution lies outside this simplex, which is indicated by \( \nu_j < 0 \), then additional negative-flash procedures are performed to find a lower dimensional tie-simplex with \( n_p < n_p^{\text{max}} \) that satisfies a global minimum of Gibbs-free energy (Iranshahr et al., 2012).

The Negative-flash approach may fail to identify the phase state correctly, if the multiphase region with \( n_p^{\text{max}} \) in the plane that intersects a given overall composition \( z \) (tie-simplex degeneration) does not exist. For such cases, the system of Eq. (3.3, 4.1-4.2) may have a non-unique solution. This disadvantage can be overcome by employing the CSAT technique in conjunction with negative-flash. In this case the CSAT algorithm can detect this degeneration prior to the use of the negative-flash, and the problem can be avoided.
CSAT-based phase identification

A tie-simplex based CSP framework was proposed to improve the performance and stability of the conventional phase behavior methods for two-phase compositional simulation (Voskov and Tchelepi, 2008). This family of methods was inspired by the Method of Characteristics (MoC) analysis developed in Entov (1997); Wang and Orr (1998). The MoC theory suggests that only a few (key) tie-simplexes determine the structure of the compositional solution in convection dominated displacements.

The CSAT method was developed following the idea of CSP for general purpose simulation based on the Natural-Variables formulation (Coats, 1980a). For this formulation, only single-phase gridblocks require stand-alone phase-stability testing, while in the two-phase region the coupled solution of Eqs. (3.1) - (3.5) is performed. The CSAT method calculates and stores the tie-simplexes that pass through a single-phase overall composition at discrete pressure levels. The CSAT procedure checks if any gridblock that requires a phase-stability test has an overall composition that is close to a tie-simplex that is already stored. If such a tie-simplex is already in the table, it is used for phase identification; if not, the CSAT parameterizes this composition, collects, and stores a set of new tie-simplexes.

It was shown by Voskov and Tchelepi (2009a) that the CSAT procedure collects a finite number of tie-simplexes for compositional problems of practical interest. The number of tie-simplex tables depends on the type of displacement and the tolerances used in CSAT. The approach was also extended for near-miscible compositional simulation (Voskov and Tchelepi, 2008), whereby CSAT detects the degeneration of a tie-simplex when miscibility is fully developed and uses this information for phase identification. It was shown that this identification strategy can improve the overall performance of the natural-variables formulation when miscibility is developed (Zaydullin et al., 2012).

Later, CSAT was extended for fully EoS-based thermal compositional simulation when more than two phases exists (Iranshahr et al., 2013). For three-phase simulation, CSAT computes the three-phase-region degeneration pressure for a given overall composition, $\mathbf{z}$, and indicates whether a three-phase negative-flash can be employed for a given $P$ and $T$. Moreover, CSAT can effectively determine the phase state of the composition using information from previously computed tie-triangles and tie-lines.
4.2 NEW BYPASS METHOD FOR PHASE-STATE IDENTIFICATION

However, it is difficult to implement a general procedure for computation of different two-phase regions outside the three-phase tie-simplex. Here, certain prior knowledge, such as the different two-phase regions outside a given tie-simplex and the tie-simplex degeneration patterns, is required. Also, one of the key assumptions of the extended CSAT method (three and more phases) is that the two-phase tie-lines must lie on the plane associated with the three-phase tie-simplex. However, in the general case, there is no guarantee that the tie-lines will not be tilted from with respect to the tie-simplex plane. The violation of this assumption can sometimes be observed for heavy-oil systems at high pressure and temperature conditions, as well as, for sour-oil compositional systems (systems with H₂S).

4.2 New bypass method for phase-state identification

In this section, we describe a new phase identification bypassing algorithm for three-phase systems; we note, however, that the method can be generalized for systems that form more than three phases.

Conventional Multiphase flash

A multiphase (three or more phases) flash procedure is required for robust phase-state identification of multicomponent mixtures when three, or more, phases may exist. The solution of the multiphase flash should satisfy the global minimum of the Gibbs-free energy. The computational cost of solving the problem rises significantly as the number of phases that may be present is three, or higher. Thus, improvements in the performance of the multiphase flash are highly desirable.

Reduced Variables (RV) is one class of methods to improve the multiphase flash. This method casts the nonlinear unknowns into a space with reduced dimensionality. This projection not only reduces the computational cost due to a reduction in the unknowns, but it also generates a smoother surface for the solution (Firoozabadi and Pan, 2002). As a result, the cost and number of nonlinear iterations can be reduced.

It was shown that the RV approach can lead to significant gains over standard
methods for the phase stability test, but the improvement in the flash (phase-split) calculations is moderate (Pan and Tchelepi, 2011; Haugen and Beckner, 2013). This makes the RV approach suitable for the natural-variables formulation where the stability of the phases needs to be tested within the global nonlinear loop. The RV method for the natural formulation was implemented and tested for two-phase EoS computations (Pan and Tchelepi, 2011). Recently, an extension of the RV method was proposed for three-phase systems (Nichita and Petitfrere, 2013).

Another type of improvement in multiphase flash strategies is the shadow-region bypass technique (Rasmussen et al., 2006). This method uses heuristics, which are based on tracking changes in $P$, $T$, and composition, to bypass the phase-stability test. While proven to be effective for a wide class of gas injection problems, this method is limited to two-phase problems.

**Bypassing of phase identification**

Our bypassing method relies on the fact that for multiphase compositional displacements in the convection-dominated (hyperbolic) limit, the phase-change shocks occur along extensions of key tie-simplexes (Voskov and Tchelepi, 2009b). In particular, the bypassing method uses information from the parametrized extensions of the key tie-simplexes.

The parametrization is performed using discretization in the space of phase fractions. In this space, the phase fractions can be negative, or greater than unity; this allows for parametrization of tie-simplex extensions. The physical boundaries of the phase-fraction space are found using the procedure described in Iranshahr et al. (2009a). Once the tie-simplex extension is discretized, a standard three-phase flash (Lucia and Feng, 2003; Petitfrere and Nichita, 2014) is used to compute the phase states at the discretization nodes. Because the tie-simplex parametrization is continuous (Iranshahr et al., 2012), if all the discretization nodes for a given cell have the same phase state, then this state can be assigned for the entire cell. On the other hand, if the phase states are different at the nodes, then the cell has a nonuniform phase state, and we proceed with the conventional three-phase flash.

This procedure is performed for the end-points of the pressure and temperature intervals, which contain the given $P$ and $T$. Then, the phase states for all pressure
and temperature end-points are compared. If the phase states are different, the conventional flash is used; otherwise, the phase state is determined. Since the number of key tie-simplexes is limited, the number of flash solves depends on the resolution of the discretization grid of the tie-simplex extension.

The negative-flash procedure is used to find the tie-simplex extension that intersects the given overall composition for the fixed pressure and temperature. Also, in a manner similar to CSAT, we compute the tie-simplex degeneration pressure and use the degenerate tie-simplex for higher pressures. The phase identification algorithm is summarized below:

- Define a regular (uniform) P-T grid.

- Project the given overall composition, \( z \), to the closest tie-simplex in the table.

- Compare the projection distance, \( d \), to the predefined tolerance. If the distance is too large, find a new tie-simplex that intersects the given overall composition using the negative-flash procedure.

- For each end-point pressure and temperature in the interval of interest:
  
  1. Discretize the tie-simplex, and its extension, in the phase-fraction space, \( \nu_j, j = 1 \ldots n_p - 1 \).
  2. Compute the phase state at the discretization nodes.
  3. Infer the phase state using information from the discretization nodes. If the nodes have different phase states, proceed with the conventional three-phase flash.

- Compare the phase states for all the pressure and temperature end-points (two end-points for pressure and two end-points for temperature). If the phase states are different, proceed with the conventional three-phase flash; otherwise, the phase state is defined.

The projection distance, \( d \), and corresponding phase fractions are obtained using the
following minimization:

$$d = \min_{\nu_j} \sum_{i=1}^{n_c} \left( z_i - \sum_{j=1}^{n_p} x_{ij}\nu_j \right)^2$$  \hspace{1cm} (4.4)

$$\sum_{j=1}^{n_p} \nu_j = 1.$$  \hspace{1cm} (4.5)

Figure 4.1 shows typical tie-simplexes (red) and the corresponding extensions for three- and four-component systems. For a three-component system, a single tie-simplex parametrizes the entire compositional space; for a four-component systems, a tie-simplex parametrizes the plane that intersects the given overall composition $z$. Here, following the standard notation, VLLE stands for vapor-liquid-liquid equilibrium, VLE denotes vapor-liquid equilibrium, etc. As can be seen, multiple two- and single-phase regions exist for these systems. Assuming a three-phase system and a fixed number of components, $n_c$, the space of phase fractions associated with a tie-simplex extension is an $n_c$-sided irregular polygon. Figure 4.2 shows the phase-fraction ($\nu$) spaces for the same three- and four-components systems. Here, the color scheme is the same as in Fig. 4.1.

Because of its simplicity, we discretize the phase-fraction space using rectilinear grids. Figures 4.3 and 4.4 demonstrate the discretized phase-fraction spaces for the two systems discussed above. At each discretization node the conventional flash is used to determine the phase states. For the cells that have the same states at all vertices, our method assigns this state for the entire cell. The grid is built adaptively; that is, the conventional flash is used to compute the phase states at vertices only if it is needed during the simulation. It is clear that finer grids allow for skipping flash calculations for larger regions of the space compared with coarser grids; however, more discretization nodes need to be computed.

In order to have a balance between phase-fraction grid resolution and the number of discretization nodes, we use adaptive coarsening of the grid. For regions that are far from phase boundaries, a coarser grid is used; whereas, a finer grid is used close to the boundaries. A rectilinear grid allows for simple implementation of this adaptive coarsening strategy. Note that for the portion of the phase-fraction space where both
4.2. NEW BYPASS METHOD FOR PHASE-STATE IDENTIFICATION

Figure 4.1: (a) \{C_1, CO_2, C_6\} at 235 K and 17 bar; (b) \{C_1, C_4, C_{20}, H_2O\} at 470 K and 150 bar (b)

Figure 4.2: Phase-fraction spaces for (a) \{C_1, CO_2, C_6\} at 235 K and 17 bar and (b) \{C_1, C_4, C_{20}, H_2O\} at 470 K and 150 bar (b)
phase fractions are positive and their sum is less than unity, the three-phase state is detected regardless of grid resolution.

Figure 4.3: Phase-fraction space discretization using coarse (a) and fine (b) grids for \{C_1, CO_2, C_6\}

### 4.3 Numerical Results

The proposed method requires only a few tie-simplexes for the parametrization of compositional displacements. This fact is based on the theory developed for hyperbolic transport of multiphase systems. Similar conclusions are valid for multidimensional systems (Voskov and Tchelepi, 2008, 2009a). Figure 4.5 shows the compositional solution paths obtained for 1D (2500x1x1 gridblocks) and 2D (50x50x1 gridblocks) simulations using \{C_1, C_4, C_20, H_2O\} system with water and water-solvent injection. It can be seen that the solution path in the 2D case deviates from the hyperbolic limit; however, the deviation (dispersion) is not significant. Note that only one tie-simplex is used to parameterize the solution path in the case of water injection, and three tie-simplexes are employed for the case of water-solvent injection.

Next, we consider two numerical examples that demonstrate the computational efficiency of the proposed method. For both examples, we use the same grid of
4.3. NUMERICAL RESULTS

Figure 4.4: Phase-fraction space discretization using coarse (a) and fine (b) grids for \{C_1, C_4, C_{20}, H_2O\}

Figure 4.5: Solution Paths for 1D and 2D displacements (a) Water Injection and (b) Water-Solvent injection
30x110x4, which was obtained by upscaling the SPE 10 reservoir model (Christie and Blunt, 2001). Moreover, the original SPE 10 permeabilities were multiplied by a factor of ten in all directions to obtain reasonable modeling time for the case of a heavy-oil reservoir (Steam-solvent injection example). For both examples, two wells are used to mimic a quarter-five-spot injection pattern, i.e., vertical production and injection wells are placed at opposite corners of the reservoir. The first example demonstrates the applicability of the bypass method for a cold CO$_2$ injection problem; whereas, the second example deals with the problem of simultaneous steam-solvent injection into a heavy-oil reservoir.

**Cold CO$_2$ injection**

We use the fluid system made up of \{C$_1$, CO$_2$, C$_6$\} presented in Iranshahr (2012). Here we inject a mixture of \{C$_1$(0.05), CO$_2$(0.95)\} at $T = 235\, K$ and $P = 70$bar into \{C$_1$(20), C$_6$(80)\} at $T = 170\, K$ and $P = 15$bar. The initial composition forms a single-phase oil ($L_1$), whereas the injection composition forms a single-phase CO$_2$-rich liquid ($L_2$). The production well is set to a constant bottom hole pressure of 2bar; at this pressure and $T = 170\, K$ the initial mixture forms a two-phase (vapor-$L_1$) fluid. The fluid properties are computed using the Soave-Redlich-Kwong (SRK) equation-of-state (Soave, 1972). The details of the EoS related properties can be found in the Appendix. The total time modeled is 1200 days. Figure 4.6 shows the CO$_2$-rich liquid ($L_2$) saturation and temperature maps for the four layers at 1200 days. It can be seen that at higher temperatures and pressures, the CO$_2$-rich liquid completely displaces the initial oil. In contrast, away from the injection well, two-phases ($L_1$-$L_2$) are present. At earlier times, two-phases (vapor-$L_1$) are observed close to the production well.

We compare the computational performance of our approach with the conventional three-phase flash (Lucia and Feng, 2003). In our implementation of the natural-variables formulation, both the phase identification bypassing algorithm and the conventional approach are used to determine the phase state only if a gridblock has less than three phases for the current Newton iteration. Due to the limitations in the software library used for this example, we run the three-phase flash algorithm to determine the phase states during the simulation. When the bypassing method is
4.3. NUMERICAL RESULTS

Figure 4.6: Simulation Results. Cold CO$_2$ injection example: CO$_2$-rich liquid Saturation (top) and Temperature Distribution (bottom) maps employed, the phase-fraction space is discretized using a 50x50 grid for a fixed ($P$, $T$) end-point pair. We note that since we use a three-component system, only one tie-simplex is needed for the bypass method. Table 4.1 summarizes the statistics for the simulations using the bypassing algorithm and conventional flash. It can be seen that when the three-phase flash is used, the phase identification constitutes 83% of the total simulation time. This is due to the large number of phase-state checks and the computational cost of the flash routine. On the other hand, phase identification using the bypassing method is responsible for 32% of the total simulation time. It can be seen that our method allows for bypassing of a significant amount of phase-state identification checks, thereby resulting in a significant reduction in the total number of three-phase flash solves (reduced by a factor of 90). As a result, the total simulation time is reduced by a factor of four.
Table 4.1: Statistics for the Cold CO₂ Injection Example

<table>
<thead>
<tr>
<th></th>
<th>Conventional Approach</th>
<th>Bypass Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase Identification Time (hr)</td>
<td>47</td>
<td>4.4</td>
</tr>
<tr>
<td>Number of Flash/Stability runs (x1000)</td>
<td>31,003</td>
<td>3,370</td>
</tr>
<tr>
<td>Number of [P, T] intervals</td>
<td>—</td>
<td>[30, 50]</td>
</tr>
<tr>
<td>Number of Tie-Simplexes Collected</td>
<td>—</td>
<td>1</td>
</tr>
<tr>
<td>Number of Discretization Nodes</td>
<td>—</td>
<td>30,391</td>
</tr>
<tr>
<td>Total Simulation Time (hr)</td>
<td>58</td>
<td>13.8</td>
</tr>
</tbody>
</table>

Steam-solvent injection into a heavy-oil reservoir

This example models steam-solvent co-injection into a heavy-oil reservoir. The oil is composed of five components: \{C₁(0.02), C₄(0.03), C₂₀(0.05), C₂₁+(0.1), H₂O(0.8)\} at \(T = 310 K\) and \(P = 30\)bar. The initial fluid is displaced by a mixture of steam and solvent of \{C₁(0.1), C₄(0.1), H₂O(0.8)\} at \(T = 540 K\) and \(P = 70\)bar. The initial composition forms a two-phase water-oil system with oil saturation equal to 78%, whereas the injection composition forms a single vapor phase. The production well is set to a constant bottom hole pressure of 1bar. For this model, we allow any component to be present in any phase (vapor, liquid oil, liquid water). The phase-equilibrium is modeled using the Peng-Robinson equation-of-state (Peng and Robinson, 1976). The details of the EoS representation can be found in the Appendix. The oil viscosity is modeled using the logarithmic mixing rule, where the viscosities are obtained using an exponential correlation (see Appendix). Figure 4.6 shows the oil saturation and temperature maps at the end of the simulation (4500 days).

The computational efficiency for the conventional approach (Petitfrere and Nichita, 2014) and the bypassing approach are presented in Table 4.2. Using the library of Petitfrere and Nichita (2014) for the conventional approach, we use phase-stability testing to determine whether a new phase can appear for a given gridblock. Here, the three-phase flash is only used to determine the phase compositions in the case of
phase appearance. For the case when the bypassing method is employed, the phase-fraction space is discretized using the 100x100 grid for a fixed \((P, T)\) end-point pair; the maximum allowed projection distance (Eq. 4.4) here is 0.02. As in the Cold CO\(_2\) injection example, when the conventional approach is employed, phase identification constitutes 40% of the computational time. For this example, the bypassing method allowed a significant number of phase identification checks to be skipped, resulting in a significant reduction in computational time. Here, only 7.4% of the phase identification runs were performed using conventional phase-stability testing; the rest of the phase state checks were bypassed. As a result, the total simulation time is reduced significantly.
### Table 4.2: Statistics for the Steam-solvent Injection Example

<table>
<thead>
<tr>
<th></th>
<th>Conventional Approach</th>
<th>Bypass Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase Identification Time (hr)</td>
<td>1.4</td>
<td>0.2</td>
</tr>
<tr>
<td>Number of Flash/Stability runs (x1000)</td>
<td>34,081</td>
<td>2,523</td>
</tr>
<tr>
<td>Number of [P, T] intervals</td>
<td>—</td>
<td>[30, 100]</td>
</tr>
<tr>
<td>Number of Tie-Simplexes Collected</td>
<td>—</td>
<td>7</td>
</tr>
<tr>
<td>Number of Discretization Nodes</td>
<td>—</td>
<td>24,546</td>
</tr>
<tr>
<td>Total Simulation Time (hr)</td>
<td>3.5</td>
<td>2.3</td>
</tr>
</tbody>
</table>

**ES-SAGD simulation**

This example demonstrates the efficiency of the bypass method for the case of ES-SAGD (Nasr and Isaacs, 2001) modeling using a fluid system with a large number of components. The reservoir model is comprised of 100x4x52 gridblocks. The total reservoir volume is \([60\times 800\times 26]\) \(m^3\) with constant gridblock dimensions. The reservoir has a constant porosity of 0.32 and homogeneous permeabilities in the I- and J-directions of 2000 mD. The vertical permeabilities vary depending on the cross section (four cross sections in a J-direction): the cross section that corresponds to \(J = 1\) has a constant vertical permeability of 200 mD; the permeabilities in the subsequent cross sections are decreased by 50 mD (the cross section that corresponds to \(J = 4\) has a constant vertical permeability of 50 mD). One SAGD pair is used for this example with a 5m distance between the injection and production horizontal wells (see Fig. 4.8). We use a uniform initial temperature of 305 K throughout the reservoir, and equilibrium a pressure of 17 bar at the top of the reservoir.

We use a 6-component model for the resident fluid description, the fluid is adapted from Badamchizadeh et al. (2011). The initial fluid is composed of \(\{C_1(1\%), nC_7(0.1\%), C_{11-28}(7\%), C_{29-45}(19\%), C_{46+}(1.9\%), H_2O(71\%)\}\). The initial oil and water saturations are 0.81 and 0.19, respectively. For the first 150 days, hot water is injected at a constant BHP of 22 bar and a temperature of 440 K. The production well is constrained at a BHP of 1 bar. After the hot water injection period, the mixture of
steam and solvent is injected at a constant pressure of 25 bar and a steam quality of 0.8; the production well is constrained at a maximum water production rate of 150 $m^3$ and a BHP of 19 bar. The injection fluid is $\{C_1(7\%), nC_7(3\%), H_2O(90\%)\}$. The simulation is performed using the EoS library presented in Petitfrere and Nichita (2014).

The results obtained after 470 days of simulation are demonstrated in Figures 4.8 where oil saturation, gas saturation, and temperature profiles are depicted for all cross sections. We observe that the gas chamber grows quite differently depending on the considered cross section. For example, the gas chamber reaches the top of the reservoir for the cross section that corresponds to $J = 1$; whereas, the chamber just starts to form for the $J = 4$ cross section.

In contrast to the previous examples, we obtained slightly different simulation results using the conventional- and bypass-based methods. The $l_2$ norm of the difference in oil saturation between the two methods is 0.038%; whereas, the maximum difference in oil saturation is 1.4% ($l_\infty = 0.014$). Here, the discrepancy in the simulation results is caused by the single occurrence of a different phase identification using two methods. During the early simulation time, a phase-stability test using conventional method indicated that one of the gridblocks needed to change its phase state; whereas, phase identification using the bypass method indicated that the mixture in the gridblock was stable. This difference in phase identification led to an additional timestep cut for the conventional method and, therefore, a very slight discrepancy in the final simulation results.

The computational efficiency of the conventional three-phase flash (Petitfrere and Nichita, 2014) and the bypassing strategy is presented in Table 4.3. Here, as in the previous example, phase-stability testing is used to determine whether the gridblock needs to change its phase state. For the bypass method, we use a grid of 100x100 for the phase-fraction space discretization. The number of pressure and temperature intervals used for the method are 10 and 60, respectively. The maximum allowed projection distance (Eq. 4.4) for the bypass method is 0.02. We observe that the phase identification time even for the conventional method constitutes only 18% of the total simulation time. This is because of the large number of components used to represent the oil, which leads to the large linear systems that need to be solved.
In fact, the global linear solver consumes 57% of the total simulation time for the conventional method.

Table 4.3 shows that the bypass method leads to a significant reduction of the phase identification time for this example. The reduction can be explained by the low number of tie-simplexes needed. However, since phase identification does not constitute the bulk of the total computational time, the overall reduction in computational time is smaller than that achieved in the previous examples (15%).

![Simulation Results](image.png)

Figure 4.8: Simulation Results. ES-SAGD example: Oil Saturation, Gas Saturation, and Temperature Distribution maps for four cross sections (J=1..4)

### 4.4 Discussion

We described a new method to bypass phase identification in three-phase thermal compositional flow simulation. During the simulation, few tie-simplexes are collected and discretized adaptively. The discretization is performed in the low-dimensional phase-fraction space. Then, the phase-states of the discretization nodes are evaluated, and the resulting phase state is inferred using the continuity of the tie-simplex parametrization. The algorithm does not require any pre-processing computations.
4.4. DISCUSSION

Table 4.3: Statistics for the ES-SAGD Example

<table>
<thead>
<tr>
<th></th>
<th>Conventional Approach</th>
<th>Bypass Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase Identification Time (hr)</td>
<td>0.84</td>
<td>0.08</td>
</tr>
<tr>
<td>Number of Flash/Stability runs (x1000)</td>
<td>48,487</td>
<td>835</td>
</tr>
<tr>
<td>Number of [P, T] intervals</td>
<td>—</td>
<td>[10, 60]</td>
</tr>
<tr>
<td>Number of Tie-Simplexes Collected</td>
<td>—</td>
<td>7</td>
</tr>
<tr>
<td>Number of Discretization Nodes</td>
<td>—</td>
<td>18,004</td>
</tr>
<tr>
<td>Total Simulation Time (hr)</td>
<td>4.7</td>
<td>4.01</td>
</tr>
</tbody>
</table>

Several numerical examples are presented for systems where three phases can coexist at equilibrium. Our numerical experiments indicate that the method is promising for speeding-up phase identification computations in three-phase compositional simulations.

The bypass approach can be easily extended to the case of more than three phases. In the case of an arbitrary number of phases, the general bypass algorithm remains the same. However, several specific parts of the algorithm still need to be generalized. These are: 1) use of generalized negative-flash to generate arbitrary dimensional \((n_p - 1)\) tie-simplexes, and 2) robust discretization of the \(n_p - 1\) dimensional phase-fraction space. These modifications are relatively straightforward, and the bypass method can therefore be used for challenging cases of four-phase (and beyond) simulation.

We also note that the proposed method is general; that is, the algorithm is independent on the actual phases that are present during simulation. The examples demonstrate the applicability of the method for complex fluid configurations. For instance, the first example dealt with a CO\(_2\)-rich liquid phase plus oil and vapor; whereas, the second and third examples dealt with steam and solvent injection. Because of this generality, we think that the bypass method can be used for extremely challenging problems, such as, gas-hydrates formation and asphaltene precipitation (solid phase modeling).
Chapter 5

Summary, Conclusions, and Future Work

Compositional simulation is necessary for designing and operating of Enhanced Oil Recovery projects. Compositional simulation involves solution of a coupled system of conservation laws, which include mass and energy conservation, with a system of thermodynamic constraints that represent instantaneous phase equilibrium of a hydrocarbon mixture. An Equation of State (EoS) model is usually employed to describe the phase behavior for two-phase isothermal simulation; whereas, the K-values approach it typically used for thermal modeling.

Compositional Space Parametrization (CSP) is a general framework for modeling compositional displacements. The framework is, to a large extent, built on the ideas that originated from the Method of Characteristics (MoC)-based theory of gas injection (Dindoruk et al., 1997; Orr et al., 1993; Orr, 2007) and tie-line based parameterization introduced by Entov et al. (2001). In this work, we developed several important concepts for the general CSP framework. The first is a new $\Gamma$–Variables formulation, where the $\gamma$-parameters are directly used in the primary variables set. This choice of primary variables allows for casting the nonlinear governing equations, including those that describe the thermodynamic phase equilibrium in tie-simplex (tie-lines for two-phase flows) space. We demonstrated that the new variables set can be beneficial in terms of nonlinear convergence for both miscible and immiscible displacements.
Another concept introduced here is discretization of the $\Gamma$-space using an adaptive, generalized octree-based technique in conjunction with hypercube triangulation. This technique allows for efficient discretization, even in the case of a large number of components. Using the octree-based discretization, we perform barycentric interpolation for the phase compositions. The analysis presented in Chapter 2 shows that this interpolation technique is quite accurate, and it allows for convergence of the CSP simulations to the EoS-based solutions upon $\Gamma$-space discretization refinement. Moreover, we demonstrated that the errors in the simulation results (i.e., saturations, phase compositions, rates, etc) can be controlled with refinement. Most importantly the errors become negligible after certain refinement levels.

Later, a general multilinear interpolation approach is introduced. Using this multilinear approach, we can represent any function in the governing conservation equations as a product of linear functions. Using this multilinear representation, we demonstrated that the general framework can be used for dynamic component lumping, or EoS tuning. Obviously, the presented example of component lumping is far from realistic; however, we can view it as preliminary step for future research. Another interesting property of the generalized framework is the separation of the primary variables achieved by employing the multilinear representation. The implications of the variables separation need to be studied further. Nevertheless, it is clear that the separation of variables can be useful for a nonlinear sequential decoupling scheme, which may be of interest in the development of a multiscale compositional simulator.

Thermal compositional simulation for modeling of EOR processes remains a challenging problem. One challenge is nonlinear convergence issues due to significant coupling between the flow equations, energy balance, and phase behavior. Another challenge is accurate phase behavior representation. Conventionally, for thermal simulations, the phase behavior is represented by employing the K-values method, which is based on the assumption of compositional independence of the K-values. In Chapter 3 we studied the impact of this assumption on the simulation results. Importantly, the presented comparisons are performed in a consistent manner. More specifically, 1) a simple 1D displacement is used to show the impact of phase behavior representation on the results, and 2) the K-values used are consistent with the corresponding
We show that the discrepancy in the simulation results between the two methods can vary from negligible to substantial depending on the fluid configuration and, more importantly, on the EOR process modeled. In cases where the discrepancy between the EoS and K-values methods is significant, the difference is attributed to violating the assumption of compositional independence of the K-values. It is clear that this violation occurs for displacements that exhibit near-miscible behavior. Therefore, EoS-based simulation is the right approach for this type of displacement. However, we note that the classical cubic EoS models are often incapable of representing the water phase and water component accurately. Therefore, more sophisticated and computationally expensive EoS models (such as the SAFT model) may be needed.

Although three-phase EoS modeling may not be important for simulation of heavy-oil thermal processes, it is absolutely essential for cases where three hydrocarbon phases are present and the displacement is miscible. One example of such a process is low-temperature CO$_2$ injection where the third CO$_2$-rich phase can form at certain pressure and temperature conditions. In this case, the three-phase EoS-based simulation is a challenging task because of the computational costs associated with three-phase thermodynamic modeling and the difficulties associated with phase labeling. In Chapter 4, we described a new method for fast three-phase phase-state identification. The method is based on the ideas developed in the two-phase CSP approach with the objective of bypassing certain phase-state identification checks. We demonstrated that the new bypass method can be quite effective for thermal EOR modeling and CO$_2$ injection at low temperatures. Although the achieved reduction in the phase identification time is substantial, the reduction in computational time is problem dependent. In the cases where the initial fluid composition lies close to the phase boundaries, the efficiency of the method is reduced.

An important property of CSP-based methods in general, and bypass methods in particular, is independence from the underlying EoS model. In other words, the CSP-based methods can accelerate phase behavior computations regardless of the EoS model used. Therefore, the bypass method can be extremely effective for cases, in which complex and computationally expensive Equations of States are employed. Another advantage of the method is its generality in terms of the maximum number
of phases present. This makes the method suitable for improving the computational speed for challenging problems, such as gas-hydrate formation and solid phase modeling.

We note that the general CSP framework presented in Chapter 2 is fully developed only for two-phase compositional simulation. Both the new bypass and generalized CSAT (Iranshahr, 2012) methods are only partial extensions of the CSP framework for cases of three and more number of phases. Therefore, a possible future research direction is to generalize the CSP the framework for arbitrary numbers of phases.
Appendix A

Properties of compositional systems used in Chapter 4

The EoS-related properties for the numerical examples presented in Chapter 4 are summarised in Tables A1-A3

Table A1: Thermodynamic Properties for the Cold CO\textsubscript{2} Injection Example

<table>
<thead>
<tr>
<th>Component</th>
<th>$T_c$ K</th>
<th>$P_c$ bar</th>
<th>$\omega$</th>
<th>$Z_c$</th>
<th>$M_w$ g/mol</th>
<th>$k_{i,C_1}$</th>
<th>$k_{i,CO_2}$</th>
<th>$k_{i,C_6}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>190.56</td>
<td>45.92</td>
<td>0.008</td>
<td>0.288</td>
<td>16.04</td>
<td>0</td>
<td>0.0933</td>
<td>0.0300</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>304.20</td>
<td>73.80</td>
<td>0.224</td>
<td>0.274</td>
<td>44.01</td>
<td>0.0933</td>
<td>0</td>
<td>0.1489</td>
</tr>
<tr>
<td>$C_6$</td>
<td>507.43</td>
<td>30.12</td>
<td>0.301</td>
<td>0.264</td>
<td>72.15</td>
<td>0.0300</td>
<td>0.1489</td>
<td>0</td>
</tr>
</tbody>
</table>

The oil viscosity in the Steam-solvent Injection example are computed using logarithmic mixing rule (A.1), where component viscosities are obtained through exponential correlation (A.2). The coefficients used in Eq. (A.2) are presented in Table A4.

\[ \ln (\mu_o) = \sum_{i=1}^{n_c} x_{i,o} \ln (\mu_{i,o}), \quad (A.1) \]

\[ \mu_i = \mu_i^* \exp (-b_i T), \quad i = 1 \ldots n_c. \quad (A.2) \]
Table A2: Thermodynamic Properties for the Steam-solvent Injection Example

<table>
<thead>
<tr>
<th>Component</th>
<th>$T_c$ K</th>
<th>$P_c$ bar</th>
<th>$\omega$</th>
<th>$M_w$ g/mol</th>
<th>$k_{i,C1}$</th>
<th>$k_{i,C4}$</th>
<th>$k_{i,C20}$</th>
<th>$k_{i,C21+}$</th>
<th>$k_{i,C_{H2O}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>190.56</td>
<td>45.92</td>
<td>0.011</td>
<td>16.04</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.05</td>
<td>0.49</td>
</tr>
<tr>
<td>$C_4$</td>
<td>425.12</td>
<td>37.96</td>
<td>0.2</td>
<td>58.12</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.51</td>
</tr>
<tr>
<td>$C_{20}$</td>
<td>768</td>
<td>10.7</td>
<td>0.865</td>
<td>282.554</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.55</td>
</tr>
<tr>
<td>$C_{21+}$</td>
<td>800.11</td>
<td>10</td>
<td>1.1</td>
<td>342</td>
<td>0.05</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.55</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>647.37</td>
<td>221.2</td>
<td>0.345</td>
<td>18.02</td>
<td>0.49</td>
<td>0.51</td>
<td>0.55</td>
<td>0.55</td>
<td>0</td>
</tr>
</tbody>
</table>

Table A3: Thermodynamic Properties for the ES-SAGD Example

<table>
<thead>
<tr>
<th>Component</th>
<th>$T_c$ K</th>
<th>$P_c$ bar</th>
<th>$\omega$</th>
<th>$M_w$ g/mol</th>
<th>$k_{i,C1}$</th>
<th>$k_{i,C4}$</th>
<th>$k_{i,C_{46+}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>190.56</td>
<td>46.04</td>
<td>0.008</td>
<td>16.04</td>
<td>0</td>
<td>0</td>
<td>0.081</td>
</tr>
<tr>
<td>$nC_7$</td>
<td>540.2</td>
<td>27.35</td>
<td>0.351</td>
<td>100.205</td>
<td>0.033</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$C_{11−28}$</td>
<td>826.12</td>
<td>17.03</td>
<td>0.721</td>
<td>305.509</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$C_{29−45}$</td>
<td>955.43</td>
<td>13.11</td>
<td>1.0</td>
<td>505.590</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$C_{46+}$</td>
<td>1222.044</td>
<td>8.34</td>
<td>1.518</td>
<td>863.92</td>
<td>0.081</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$H_2O$</td>
<td>647.37</td>
<td>221.2</td>
<td>0.351</td>
<td>18.02</td>
<td>0.081</td>
<td>0.165</td>
<td></td>
</tr>
</tbody>
</table>
The component oil viscosities for the ES-SAGD example are defined by a tabulated data presented in Table A5.

Table A4: Viscosity Correlation Coefficients

<table>
<thead>
<tr>
<th>Component</th>
<th>$\mu_i^*$</th>
<th>$b_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>100</td>
<td>0.02</td>
</tr>
<tr>
<td>$C_4$</td>
<td>200</td>
<td>0.02</td>
</tr>
<tr>
<td>$C_{20}$</td>
<td>2000</td>
<td>0.02</td>
</tr>
<tr>
<td>$C_{21+}$</td>
<td>100000</td>
<td>0.02</td>
</tr>
</tbody>
</table>
### Table A5: Components' Viscosities for the ES-SAGD example

<table>
<thead>
<tr>
<th>T(K)</th>
<th>$C_1$</th>
<th>$nC_7$</th>
<th>$C_{11-28}$</th>
<th>$C_{29-45}$</th>
<th>$C_{46+}$</th>
<th>$H_2O$</th>
</tr>
</thead>
<tbody>
<tr>
<td>278.15</td>
<td>0.015307</td>
<td>0.80102</td>
<td>204.03</td>
<td>96236</td>
<td>4.48E+13</td>
<td>1.10129497</td>
</tr>
<tr>
<td>293.939</td>
<td>0.021105</td>
<td>0.60865</td>
<td>71.302</td>
<td>13925</td>
<td>4.25E+11</td>
<td>0.82183203</td>
</tr>
<tr>
<td>309.729</td>
<td>0.02837</td>
<td>0.48804</td>
<td>30.421</td>
<td>2874.4</td>
<td>9108500000</td>
<td>0.63185301</td>
</tr>
<tr>
<td>325.518</td>
<td>0.036809</td>
<td>0.39639</td>
<td>15.213</td>
<td>786.77</td>
<td>373370000</td>
<td>0.49834614</td>
</tr>
<tr>
<td>341.308</td>
<td>0.046112</td>
<td>0.32389</td>
<td>8.6231</td>
<td>269.37</td>
<td>25761000</td>
<td>0.40177045</td>
</tr>
<tr>
<td>357.097</td>
<td>0.056096</td>
<td>0.26959</td>
<td>5.3887</td>
<td>110.08</td>
<td>2702900</td>
<td>0.33014401</td>
</tr>
<tr>
<td>372.887</td>
<td>0.066604</td>
<td>0.22768</td>
<td>3.6408</td>
<td>51.887</td>
<td>399100</td>
<td>0.27583263</td>
</tr>
<tr>
<td>388.676</td>
<td>0.077523</td>
<td>0.19449</td>
<td>2.6195</td>
<td>27.468</td>
<td>78015</td>
<td>0.2338484</td>
</tr>
<tr>
<td>404.466</td>
<td>0.088777</td>
<td>0.16763</td>
<td>1.9835</td>
<td>15.998</td>
<td>19233</td>
<td>0.20082505</td>
</tr>
<tr>
<td>420.255</td>
<td>0.10032</td>
<td>0.14548</td>
<td>1.5658</td>
<td>10.087</td>
<td>5752.2</td>
<td>0.17445098</td>
</tr>
<tr>
<td>436.045</td>
<td>0.11208</td>
<td>0.12688</td>
<td>1.2792</td>
<td>6.7963</td>
<td>2023.2</td>
<td>0.15309235</td>
</tr>
<tr>
<td>451.834</td>
<td>0.12397</td>
<td>0.11098</td>
<td>1.075</td>
<td>4.8439</td>
<td>815.97</td>
<td>0.13558172</td>
</tr>
<tr>
<td>467.624</td>
<td>0.13584</td>
<td>0.097083</td>
<td>0.92478</td>
<td>3.6215</td>
<td>369.72</td>
<td>0.12106206</td>
</tr>
<tr>
<td>483.413</td>
<td>0.14746</td>
<td>0.084581</td>
<td>0.81147</td>
<td>2.8211</td>
<td>185.1</td>
<td>0.10890089</td>
</tr>
<tr>
<td>499.203</td>
<td>0.15851</td>
<td>0.072769</td>
<td>0.72442</td>
<td>2.2778</td>
<td>101.06</td>
<td>0.09861898</td>
</tr>
<tr>
<td>514.992</td>
<td>0.16863</td>
<td>0.060262</td>
<td>0.65801</td>
<td>1.9015</td>
<td>59.622</td>
<td>0.08985313</td>
</tr>
<tr>
<td>530.782</td>
<td>0.18261</td>
<td>0.23982</td>
<td>0.50526</td>
<td>1.3483</td>
<td>31.066</td>
<td>0.08232065</td>
</tr>
</tbody>
</table>
Nomenclature

Abbreviations

$\gamma$  Tie-line parameter
$\beta$  Barycentric coordinates
$x_k^*$  Phase compositions associated with $k^{th}$ supporting point
$k$  Permeability tensor
$\gamma_k^*$  Coordinates of $k^{th}$ supporting point
$\kappa$  Thermal Conduction
$\mu_j$  Viscosity of phase $j$
$\nu_j$  Fraction (by mole) of phase $j$
$\omega$  Acentric factor
$\phi$  Porosity
$f_{i,j}$  Fugacity of component $i$ in phase $j$
$H_j$  Enthalpy of phase $j$
$K_i$  Equilibrium ratio of component $i$ (K-value)
$k_{rj}$  Relative permeability of phase $j$
$L$  Liquid phase fraction (by mole)
$n_c$  Number of components
$n_p$  Number of phases
$P$  Pressure
$P_c$  Critical pressure
$q_j$  Source/sink of phase $j$
$S_j$  Saturation of phase $j$
$T$  Temperature
$T_c$  Critical temperature
$U_j$ Internal energy of phase $j$

$u_j$ Darcy velocity of phase $j$

$U_R$ Rock Internal energy

$V_\gamma$ Maximum distance in the octree hyper-cube

$x_{i,j}$ Composition of component $i$ in phase $j$

$z_i$ Overall composition of component $i$
Bibliography


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Equilibria, 283(1-2), 1 – 11.


