DIRECT DISCRETIZATION OF THE TIE-LINE SPACE FOR COMPOSITIONAL FLOW SIMULATION

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By
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I certify that I have read this report and that in my opinion it is fully adequate, in scope and in quality, as partial fulfillment of the degree of Master of Science in Energy Resources Engineering.

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Abstract

We present a new and efficient methodology for the explicit representation of thermodynamic phase behavior associated with multicomponent two-phase flow in porous media. The method is based on interpolation in the discretized tie-line (Γ) space. Since a large number of supporting points may be required needed for direct discretization of the Γ−space, the discretization is performed adaptively during the simulation. A procedure based on the generalization of the octree data structure is proposed for adaptive discretization of the Γ−space, which can be of arbitrary dimension. Then, the tie-lines space is tessellated using Delaunay triangulation and the natural-neighbor interpolation technique is used inside a simplex. It is important to note that the EoS computations need to performed only for a limited number of supporting points and that a different EoS model (or EoS-free model) can be used for different regions of the Γ-space.

Based on this method, a new nonlinear formulation for general purpose compositional simulation for both immiscible and miscible displacements is proposed. The representation of the sub-critical space is based on the tie-line (γ) variables; whereas the super-critical space is parametrized using overall compositions as nonlinear unknowns. Variable substitution is based on the parametrized critical tie-line and the Minimal Critical Pressure criterion.

Numerical experiments indicate that the proposed approach reduces the cost of the thermodynamic related computations quite substantially compared with the standard methods.
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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 significant.

Compositional models are described by a set of nonlinear equations that include mass conservation equations and thermodynamic equilibrium constraints. The phase behavior of a hydrocarbon mixture is usually described using an Equation of State (EoS) model (Coats, 1980; Aziz and Wong, 1989). The EoS-based phase behavior computations can be split into two procedures: phase-stability assessment (Michelsen, 1982a) and flash computations (Michelsen, 1982b). The EoS computations must be performed for each computational cell (gridblock) for each Newton iteration; therefore, these computations consume a significant fraction of the total simulation time.

Another important aspect of any compositional model is the choice of the primary variables used to solve the governing equations. There are several popular choices for the primary variables, and 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, 1980) 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 et al., 2009).

Several different approaches have been proposed to improve the efficiency of phase
behavior computations in compositional flow simulation. In cases where the phase behavior is a weak function of composition, a model based on constant K-values can be used, in which the K-values depend on pressure and temperature only (Bolling, 1987). This approach allows for extremely efficient thermodynamic computations, but is accurate only for low pressures and temperatures. The standard K-value approach is not adequate for problems involving complex compositional effects, such as multi-contact miscible displacements. Another possibility is to limit the number of components and represent the phase behavior using simplified relations (Pope and Nelson, 1972; Todd and Longstaff, 1972).

Another approach for phase-behavior representation of two-phase compositional systems was suggested by Entov et al. (2001). Their method is based on projection of the original compositional problem into tie-line (Γ) space, where simple polynomial approximations of the tie-line space are used to capture the important features of the two-phase region (Voskov, 2002). Later, Voskov and Tchelepi (2009c) showed that linear interpolation in the discretized tie-line space can be used to represent thermodynamic phase behavior. They refer the approach to as Compositional Space Parameterization (CSP) based flow simulation.

The CSP approach is based on parameterizing the entire compositional space. It was shown that for purely hyperbolic 1D problems, projection of the solution into 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, 2009b) that for compressible, multi-dimensional displacements in porous media, projection of the solution in tie-line space is nearly invariant. However, a larger number of tie-lines may have to be collected due to the numerical dispersion associated with the numerical solutions.

The CSP approach motivated the development of the Compositional Space Adaptive Tabulation (CSAT) method (Voskov and Tchelepi, 2009b, 2008). The CSAT method is based on the fact that gas injection displacement processes involve a limited number of (key) tie-lines (Bedrikovetsky and Chumak, 1992; Franklin M. Orr, 2007). The CSAT approach adaptively stores discrete tie-lines (i.e., phase compositions) during a simulation. The collected tie-lines are used to look-up the phase
state of the mixture, thus replacing 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 simulator up to the time of interest. CSAT is adaptive by construction; as a result, a standard EOS solver is needed as new regions of the compositional space are encountered by the simulation.

When the natural-variables formulation is used, the phase-stability tests make 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 (Firoozabadi and Pan, 2002) have been developed. Another interesting approach is the so-called shadow region method (Rasmussen et al., 2006) for bypassing some stability tests during a simulation. Pan and Tchelepi (2011) combined phase-stability and bypassing, both based on reduced variables, and they demonstrated that the combined strategy is very effective in reducing the overall cost of EoS computations in general-purpose compositional simulation.

In this work, we develop an adaptive compositional space parameterization (ACSP) approach, which is based on adaptive interpolation in the discretized tie-line space. This approach allows for continuous representation of the phase envelope (boundary) as a function of composition and pressure. The governing equations here are cast in terms of the tie-line parameters ($\gamma$), which allows for decoupling of the elliptic flow problem (pressure) and hyperbolic transport problem ($\gamma$). The applicability of ACSP is demonstrated for several miscible and immiscible gas injection problems.
Chapter 2

Tie-Simplex Space Discretization

2.1 Conventional approach for compositional flow simulation

The system of equations for a two-phase isothermal compositional problem can be written as:

$$\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{2} x_{i,j} \rho_j S_j \right) - \text{div} \sum_{j=1}^{2} x_{i,j} \rho_j \left( k r_j \frac{\mu_j}{\mu_j} \nabla p \right) + \sum_{j=1}^{2} x_{i,j} \rho_j q_j = 0, \ i = 1, \ldots, n_c.$$  \hspace{1cm} (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, $r_j$ is relative permeability, $\mu_j$ is the phase viscosity and $p$ is pressure.

Instantaneous thermodynamic equilibrium is the usual assumption for the compositional model. The thermodynamic relations are usually dealt with using two different 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.

Both of these approaches have their own advantages and drawbacks (Voskov et al., 2009).

The overall composition, $z$, for a two-phase system can be represented as a linear combination of phase fractions $x_{i,j}$:

$$z_i = x_{i,o}L + x_{i,g}(1 - L), \quad i = 1, \ldots, n_c$$

$$L = S_o\rho_o/(S_o\rho_o + S_g\rho_g),$$

where $L$ is the fraction of the liquid (oil) phase. Then, the accumulation term of (2.1) can be expressed as

$$\phi \sum_j x_{i,j}\rho_j S_j = \phi \rho z_i,$$

where $\rho = S_o\rho_o + S_g\rho_g$.

Since a mixture $z$ at a given $p$ and $T$ in any grid-cell can be in a single (vapor or liquid) or a two-phase state, the phase equilibrium computations involve a two-step procedure:

- For any grid cell which has a single phase state, the phase stability test is performed (Michelsen, 1982a) to check weather the current state will switch to a different single-phase or to a two-phase state.

- For any grid cell which has a two-phase state, flash calculation is performed (Whitson and Michelsen, 1989) to compute the phase compositions at equilibrium.

**Stability test**

To determine the phase state (single-phase, or two-phase) of composition $z_i$, the stability of both the liquid and gas phases is checked. The stability criterion expressed in terms of the mole fraction and fugacity coefficients $\Phi_i = f_i/(x_{i,g}p)$ can be written
as (Michelsen, 1982a)

\[
\sum_{i=1}^{N} (\ln x_{i,g} + \ln \Phi_i(x_g) - \ln z_i - \ln \Phi_i(z)) \geq 0.
\]  

(2.5)

It can be shown that the minimum of the left hand side is a stationary point satisfying

\[
\ln x_{i,g} + \ln \Phi_i(x_g) - \ln z_i - \ln \Phi_i(z) = \eta,
\]  

(2.6)

where \(\eta\) is independent of \(i\). Now, we can write

\[
\ln Y_i = \ln x_{i,g} - \eta \Leftrightarrow x_{i,g} = Y_i e^\eta
\]  

(2.7)

and equation (2.6) can be rewritten as

\[
F_i \equiv \ln Y_i + \ln \Phi_i(x_g) - \ln z_i - \ln \Phi_i(z) = 0, \quad i = 1, \ldots, N.
\]  

(2.8)

Introducing \(K_i = Y_i / z_i\) into equation (2.8), we get

\[
F_i \equiv \ln K_i + \ln \Phi_i(x_g) - \ln \Phi_i(x) = 0, \quad i = 1, \ldots, N
\]  

(2.9)

This nonlinear system of equations must be solved for the unknowns \(\alpha_i = \ln K_i\).

We use the following initial guess for \(K_i\) (Michelsen, 1982a)

\[
p_{si} = e^{5.373(1+\omega_i)(1-T_{ci}/T)} p_{ci}, \quad K_i = p_{si} / p,
\]  

(2.10)

where \(p_{ci}\) and \(T_{ci}\) denote the critical pressure and temperature for component \(i\), and \(\omega_i\) is the acentric factor. An initial estimate for \(X_i\) can be calculated as follows:

\[
X_i = z_i / K_i.
\]  

(2.11)

For the liquid-phase check, the initial guess can be found from

\[
Y_i = z_i K_i.
\]  

(2.12)
The phase fugacity can be calculated as:

$$\ln f_{iV} = \ln(x_{i,g}p) - \ln(Z - B)$$  \hspace{1cm} (2.13)

$$+ \frac{A}{(m_1 - m_2)B} \left( \frac{2}{A} \sum_{j=1}^{N} x_{j,g} A_{ij} - \frac{B_i}{B} \right) \ln \frac{Z + m_2 B}{Z + m_1 B} + \frac{B_i}{B} (Z - 1),$$

The phase fugacities are substituted into (2.8) and iterations are performed until convergence. If $\sum_{i=1}^{N} Y_i < 0$ based on (2.6), the current phase state is stable. If both single-phase states are unstable, a flash procedure is performed.

**Flash calculations**

The flash calculations involve solving the following nonlinear system

$$z_i - Lx_{i,o} - (1 - L)x_{i,g} = 0, \quad i = 1, \ldots, n_c$$  \hspace{1cm} (2.14)

$$f_{i,o}(p, T, x_o) - f_{i,g}(p, T, x_g) = 0, \quad i = 1, \ldots, n_c$$  \hspace{1cm} (2.15)

$$\sum_{i=1}^{n_c} (x_{i,o} - x_{i,g}) = 0.$$  \hspace{1cm} (2.16)

Here $f_{i,g}$ and $f_{i,o}$ represent the fugacity of component $i$ in the vapor and liquid phases, respectively. For a given $p$, $T$, and $z$, the unknowns are $x_{i,o}$, $x_{i,g}$ and $L$. The solution of this system usually involves the combination 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 - 2.16) 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, 1980) and *Molar* (Chien et al., 1985; Wang et al., 1997) *Variables* were used to perform the conventional compositional simulations.
1. **The Natural Variables** formulation employs the following set of unknowns (number of unknowns is indicated in square brackets):

   - \( p \) – pressure [1],
   - \( S_g \), – phase saturations [1],
   - \( x_{i,j} \) – phase saturations \([2n_c]\),

   The phase fraction \( L \) is obtained from the phase saturations and densities:
   \[
   L = \frac{S_o \rho_o}{\sum_{j=o,g} S_j \rho_j}.
   \] (2.17)

   The overall composition \( z \) can be obtained from (2.2); for single-phase mixtures \( z = x_p \), where \( p \) is the phase state of the mixture.

   For this formulation, the system of equations (2.1) is chosen as the primary equation set; the primary unknowns are \( p \), \( S_g \), and \( n_c - 2 \) phase fractions, \( x_{i,j} \).

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

   - \( p \) – pressure [1],
   - \( L \), – liquid phase fraction[1],
   - \( ln(K_i) \) – phase composition for the gas phase \([n_c]\),
   - \( z_i \) – overall composition \([n_c]\),

   The phase compositions are obtained from the definition of the \( K \) – values and Eq. (2.2):
   \[
   x_{i,o} = \frac{z_i}{L + K(1 - L)},
   \] (2.18)
   \[
   x_{i,g} = K_i x_{i,o}.
   \] (2.19)

   The EoS is used to compute phase densities \( \rho_j = \rho_j(p, T, x_{i,j}) \); the phase saturations can be found from (2.17).
Here, the system of equations (2.1) is used as the primary equations set. Primary variables are: \( p \) and \( n_c - 1 \) overall compositions – \( z_i \).

The fully implicit method (FIM) is used throughout this report to solve the system of equations (2.1) for a given set of unknowns. Specifically, the Newton-Raphson method is used to linearize the system of nonlinear equations, in which a Jacobian system is assembled and solved for each nonlinear iteration. The flow equations account for fluxes across cell boundaries; as a result, these equations depend on the unknowns in adjacent grid blocks. The relationship between the cell and its neighbors depends on the specific discretization scheme used. Consistent with their wide use in the general-purpose simulation community, the two-point flux approximation (TPFA) and single-point phase-based upstream weighting were used here.

### 2.2 Parametrization of the sub-critical space

Parametrization of the compositional space using the tie-line parameter \( \gamma \) was discussed by Entov (1997); Voskov and Tchelepi (2009b). The important property of the parametrization is the invariance of \( \gamma \) with respect to the hydrodynamical problem (Entov et al., 2001). In this work, the parametrized space is directly used for representation of the thermodynamic phase behavior associated with multicomponent two-phase flow simulation.

As discussed in the previous section, for a given overall composition \( z \) one can find the corresponding fractions in the vapor and liquid phases, \( x_{i,j} \), by performing a two-phase flash. A line which connects the fractions on the bubble- and dew-point curves is called a tie-line (see Figure 2.1). Here, we assume that tie-lines never intersect inside the compositional space. Therefore, each tie-line can be uniquely parametrized by a \( \gamma \) parameter that is constant along the tie-line. The set of these parameters forms the \( \Gamma \)-space. Here, \( \gamma \) is defined as a set of coordinates associated with the center point of the tie-line (i.e., \( \gamma_i = (x_{i,o} + y_{i,o})/2 \)). Thus, each tie-line in the compositional space has a corresponding unique \( \gamma \) in the \( \Gamma \)-space. The dimension of the parameterized space depends on the number of components and phases. For a two-phase system, it is equal to \([n_c - 2]\).
Figure 2.1: Tie-lines and corresponding $\gamma$ for the three-component system $\{C_1, C_{10}, CO_2\}$

Voskov and Tchelepi (2009b) proposed an approach for the parametrization of the compositional space based on the standard compositional variable set $\{p, z\}$. 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 (2.15) is linear within any simplex of the discretized space. This linearity assumption requires very small simplexes, and that leads to an excessively large number of simplexes to cover the compositional space (Zaydullin et al., 2010). Figure 2.2 shows comparisons between the EoS-based solution (saturation) for 1D immiscible gas displacement of a four-component system and the solution based on tie-line interpolation for two different sizes of simplexes. It can be seen that the results for larger simplexes have larger error compared with the EoS-based solution. Moreover, due to the assumption of linearity of (2.15), the saturation field obtained with the larger simplexes displays a non-monotonic saturation profile.

In this work, the standard variable set $\{z_i, i = 1, \ldots, n_c - 1\}$ is replaced by a new set, namely, $\{L, \gamma_i, i = 1, \ldots, n_c - 2\}$. Here, $L$ is the liquid phase fraction and $\gamma$ is the vector of the tie-line parameter. We refer to this variables set as $Gamma Variables$.

Based on this set, a new framework for phase equilibrium computations is introduced. Given the tie-line parameter, $\gamma$, pressure, and temperature, the proposed
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Figure 2.2: Representation of saturation distribution for four component system \{C_1, C_{10}, C_4, CO_2\} for large (a) and small (b) size of simplexes; here EoS-based solution is shown in solid line, CSP solution in circles.

phase equilibrium procedure returns the liquid and vapor fractions, phase compositions, and all necessary derivatives.

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. Based on the supporting \(\gamma\) points, the \(\Gamma\)-space is tessellated.

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 fractions 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.

2.2.1 Adaptive interpolation in parameterized space

Since a tie-line is a continuous function of \(p, T\) and composition \(z\) (Iranshahr et al., 2009), interpolation can be used for computation of a tie-line inside a simplex for the...
pressure interval. The interpolation algorithm was originally proposed by Voskov and Tchelepi (2009c) for the standard compositional variables set \( \{p, z\} \). Recently, the original algorithm is modified by Zaydullin et al. (2010) in order to use the Gamma Variables for the representation of the compositional space.

To represent a tie-line as a function of the parameter \( \gamma \), natural-neighbor interpolation scheme (Sibson, 1981) was used, where the \( n \)-dimensional \( (n = n_c - 2) \). \( \Gamma \)-space was triangulated using Delaunay tessellation. For the tessellation of scattered data, linear interpolation of any point inside a simplex was performed (Figure 2.3), namely:

\[
\gamma_i = \sum_{k=1}^{n+1} \lambda_k \gamma^*_{k,i}, \quad i = 1, \ldots, n
\] (2.20)

where the \( \lambda_k \) 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. The system of linear equations (2.20) can be rewritten in matrix notation as follows:

\[
\begin{bmatrix}
\Gamma \\
e
\end{bmatrix}
\lambda =
\begin{bmatrix}
\gamma \\
1
\end{bmatrix}.
\] (2.21)

Here, \( \Gamma \) is a matrix of the coordinates of all the vertices \( (n + 1) \), and \( e \) is the unit vector, which arises from the constraint on the sum of the barycenter coordinates.

By solving the linear system (2.21), one can determine the barycenter coordinates of the interpolated point. Since the matrix \( \Gamma \) does not depend on the coordinates of the interpolated point \( \gamma \), the barycenter coordinate is a linear function of the tie-parameter \( \gamma \). Therefore, inside each simplex, the derivatives of \( \lambda_k \), \( k = 1, \ldots, n + 1 \) with respect to \( \gamma_i \), \( i = 1, \ldots, n \) are constants, i.e \( \frac{\partial \lambda_k}{\partial \gamma} = \text{const} \), \( k = 1, \ldots, n + 1 \).

Knowing the barycenter coordinates of the interpolated point, the mole fractions
Figure 2.3: Interpolation simplex for four component system
for the end points for the pressure interval of interest can be computed as follows:

\[
x_{i,j}^1 = \sum_{k=1}^{n+1} \left( x_{i,j}^* (p_1) \right)_k \lambda_k, \quad i = 1, \ldots, n_c \quad j = \{o, g\}, \tag{2.22}
\]

\[
x_{i,j}^2 = \sum_{k=1}^{n+1} \left( x_{i,j}^* (p_2) \right)_k \lambda_k, \quad i = 1, \ldots, n_c \quad j = \{o, g\}. \tag{2.23}
\]

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

\[
x_{i,j} = x_{i,j}^1 + \frac{x_{i,j}^2 - x_{i,j}^1}{p_2 - p_1} (p - p_1) \quad i = 1, \ldots, n_c \quad j = \{o, g\}. \tag{2.24}
\]

Since linear interpolation in both pressure and composition is used for phase fraction computations, derivatives of \( x_{i,j} \) with respect to all unknowns in the set are constant:

\[
\frac{\partial x_{i,j}}{\partial \gamma} = \text{const}, \tag{2.25}
\]

\[
\frac{\partial x_{i,j}}{\partial p} = \text{const}. \tag{2.26}
\]

Figure 2.4 shows the phase envelope for a four-component system \( \{C_1, C_{10}, C_4, CO_2\} \) computed using a standard EoS procedure and our adaptive interpolation. The two surfaces match quite well, and the largest interpolation error (5%) is observed in the vicinity of the critical point. The corresponding triangulated \( \Gamma \)-space is shown in Figure 2.5. It can be seen that a small number of supporting tie-lines (red dots) is needed for the representation of the two-phase envelope.

Figures 2.6 and 2.7 show the compositional and corresponding \( \Gamma \) spaces for another four-component system. As in the previous case, the interpolation error is not significant (4%), and even fewer supporting points are needed for the parametrization.
Figure 2.4: Compositional space for the four-component system \( \{ C_1, C_{10}, C_4, CO_2 \} \). Red and blue are the dew and bubble points surfaces obtained with standard negative-flash. Black and yellow are the dew and bubble points surfaces obtained with adaptive interpolation.

Figure 2.5: \( \Gamma \)-space for the four component system \( \{ C_1, C_{10}, C_4, CO_2 \} \). Red dots are the supporting tie-lines. Green dots are the interpolated tie-lines.
Figure 2.6: Compositional space for the four-component system \( \{N_2, C_6, C_8, CO_2\} \). Red and blue are the dew and bubble points surfaces obtained with standard negative-flash. Black and yellow are the dew and bubble points surfaces obtained with adaptive interpolation.

Figure 2.7: \( \Gamma \)-space for the four-component system \( \{N_2, C_6, C_8, CO_2\} \). Red dots are the supporting tie-lines. Green dots are the interpolated tie-lines.
2.2.2 Tessellation of the tie-line space

As can be seen in Figures 2.5 and 2.7, accurate tessellation is needed in order to perform interpolation. For this purpose, the generalized octree data structure was used. An octree is a data structure in which each node has exactly eight children (Eberhardt et al., 2010). The two-dimensional analogue of an octree is a quadtree—a tree data structure in which each node has exactly four children. Figures 2.8 shows quadtree and octree examples. Two major advantages of an octree (as well as arbitrary dimensional generalized octree) are: high memory efficiency because the tree’s size is limited and very fast searches throughout the tree. These advantages make an octree structure attractive for our adaptive interpolation. Since in the general case, the dimension of the Γ-space can be greater than three, an octree data structure was generalized for spaces of arbitrary dimension. Note that Delaunay triangulation is used inside each hyper-cube (see Figure 2.9). The advantages of the proposed algorithm can be summarized as follows:

- The natural-neighbor interpolation requires only \(n_c - 1\) supporting points; whereas, polylinear interpolation (generalization of trilinear interpolation) involves \(2^{n_c - 1}\) supporting vertexes for the interpolation.

Figure 2.8: Quadtree (left) and Octree (right) examples.
• 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.

2.2.3 Flash calculation in parameterized space

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

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

\[
\gamma_i - g_i(x_o, x_g) = 0, \quad i = 1, \ldots, n_c - 2
\]  
\[ (2.27) \]

\[
x_{o,i} \zeta_{i,o}(p, T, x_o) - x_{g,i} \zeta_{i,g}(p, T, x_g) = 0, \quad i = 1, \ldots, n_c
\]  
\[ (2.28) \]

\[
\sum_{i=1}^{n_c} x_{i,j} - 1 = 0, \quad j = o, g.
\]  
\[ (2.29) \]

The definition of \( g_i \) depends on how one determines \( \gamma_i \). Here, the center point of the
tie-line is used as the tie-line parameter, i.e. \( g_i = (x_{i,o} + x_{i,g})/2, \ i = 1, \ldots, n_c - 2 \). So, for given \( p, T \) and \( \gamma \), the corresponding \( x_o \) and \( x_g \) need to be obtained.

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

\[
K_i = \frac{x_{i,g}}{x_{i,o}} = \frac{p_{c,i}}{p} \exp \left( 5.37(1 + w_i) \left( 1 - \frac{T_c}{T} \right) \right), \ \forall i = 1, \ldots, n_c. \quad (2.30)
\]

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

\[
x_{i,o} = \frac{2\gamma_i}{K_i + 1}, \ \forall i = 1, \ldots, n_c - 2, \quad (2.31)
\]

\[
x_{i,g} = K_i x_{i,o}, \ \forall i = 1, \ldots, n_c - 2. \quad (2.32)
\]

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:

\[
(K_{n_c-1} - K_{n_c}) x_{n_c,o} = K_{n_c-1} x_{n_c,o} - K_{n_c} x_{n_c,o} = K_{n_c-1} x_{n_c,o} - x_{n_c,g} \quad (2.33)
\]

which can be rearranged as:

\[
K_{n_c-1} x_{n_c,o} - x_{n_c,g} = (K_{n_c-1} x_{n_c,o} + x_{n_c-1,g}) - x_{n_c-1,g} - x_{n_c,g}
= K_{n_c-1} \left( x_{n_c,o} + x_{n_c-1,g} \right) - x_{n_c-1,g} - x_{n_c,g}. \quad (2.34)
\]

Taking in account equation (2.29), the last relation can be written as:

\[
K_{n_c-1} x_{n_c,o} - x_{n_c,g} = K_{n_c-1} \left( 1 - \sum_{i=1}^{n_c-2} x_{i,o} \right) + \sum_{i=1}^{n_c-2} x_{i,g} - 1 \quad (2.35)
\]
Combining (2.33) and (2.35) leads to:

\[ x_{n_c,o} = \frac{\sum_{i=1}^{n_c-2} x_{i,g} + K_{n_c-1} \left( 1 - \sum_{i=1}^{n_c-2} x_{i,o} \right) - 1}{K_{n_c-1} - K_{n_c}}. \] (2.36)

The other compositions can be found from (2.29) and the K-value definition. Next, the \( x_{i,j} \) are substituted into the fugacities, Eq.(2.28), and the \( K \)-values are updated as follows:

\[ K^{(m)}_i = \frac{\Phi^{-1}_i(x_{i,o})}{\Phi^{-1}_i(x_{i,g})}, \] (2.37)

Here \( m \) is the SSI iteration number and \( \Phi_i \) is the fugacity coefficient of component \( i \).

The SSI iterations are repeated until convergence is achieved. SSI can be accelerated by switching to the Newton method at some threshold value of the residual. Such an approach requires linearization of system (2.27)-(2.29) for each Newton iteration and updating the nonlinear unknowns, \( x_o \) and \( x_g \), based on the solution of the linear system until convergence is reached.

### 2.3 Super-critical space representation

Accurate representation of the super-critical region is essential for modeling miscible gas-injection processes. The super-critical space cannot be parametrized by tie-lines simply because tie-lines do not exist in this space. Here, we use the Adaptive Super-Critical State Criteria (SSC) introduced by Voskov and Tchelepi (2008, 2009a) and variable switching during the simulation.

#### 2.3.1 Representation of the near-critical region

The interpolation algorithm described above can be used, as long as, the solution path is below the hyper-surface of critical tie-lines (Voskov and Tchelepi, 2008). However, in compositional problems of practical interest, part of the solution path may lie in the super-critical region. This section discusses the extension of the adaptive
parameterization approach for representation of the portion of the sub-critical space close to the critical locus.

The main idea is based on the fact that for a fixed temperature, $T$, a unique critical tie-line passes through each point in the compositional space (Voskov and Tchelepi, 2009a; Iranshahr et al., 2010). Each critical tie-line corresponds to a Minimal Critical Pressure (MCP) – the minimal pressure at which the length of a tie-line is close to zero (see Figure 2.10). As a result, part of the sub-critical region close to the critical locus can be parameterized by the critical tie-lines with different MCPs. Interpolation

![Figure 2.10: Minimal Critical Pressure for three component system](image)

in the super critical-region can be performed as follows:

- For each supporting point, calculate the MCP.
- Find the simplex that contains the current $\gamma$.
- If the current pressure is above the MCP of any vertex, use the critical tie-line defined at these vertices for interpolation.
• Otherwise, use the standard tie-line interpolation described above.

This algorithm was tested for several compositional systems of practical interest. Fig. 2.11-a shows an example of interpolation in a large ($\approx 1/2$ of compositional space) simplex using a four-component system $\{C_1, C_{10}, C_4, CO_2\}$. The pressure was changed continuously and the corresponding interpolation errors using our Gamma-based flash procedure were computed. Fig. 2.11-b represents the interpolation error and the tie-line length versus pressure. As the pressure increases, the length of the tie-line goes to zero smoothly. The EOS-based tie-line and the interpolated tie-line are in good agreement, even though the size of the simplex is quite large. Moreover, there are no jumps in the pressure values that correspond to the MCP of the supporting point. This fact indicates that interpolation in the presence of critical tie-lines is reasonably accurate.

Figure 2.11: Adaptive interpolation for System 1: (a) simplex in the $\Gamma$-space with corresponding MCP and (b) the interpolation error and tie-line length vs pressure.
2.3.2 Variables substitution strategy for super-critical space representation

As mentioned earlier, the super-critical space cannot be parametrized 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 Gamma Variables set cannot be used to represent the super-critical region. However, it is convenient to parametrize the space by using pressure and overall compositions, i.e. \{p, z\}, as a set of primary unknowns. Thus, two different sets of unknowns are used to parametrize the entire compositional space: The Gamma Variables and \{p, z\} for representing of the sub- and super-critical spaces, respectively.

Figure 2.12 shows the parameterization used in the Natural Variables formulation. Here, three different set of unknowns are used, namely: \{p, S_g, x_o, x_g\} for the two-phase region, \{p, x_g\} for single-phase gas and \{p, x_o\} for single-phase liquid. Figure 2.13 presents the parametrization based on the Gamma Variables set; two different sets of unknowns are used for the representation of sub- and super-critical spaces.

Figure 2.12: Phase diagram used in the Natural Variables formulation

As Figure 2.12 indicates, the Natural Variables formulation does not “see” the
Figure 2.13: Phase diagram used in the Gamma Variables formulation

difference between 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 Gamma Variables formulation, on the other hand, distinguishes between the super- and sub-critical compositions in an effective manner.

In order to use the Gamma Variables formulation, robust switching criteria between the two sets of unknowns are required. In this work, the Adaptive SSC criterion is used to determine whether a composition lies in the sub- or super-critical regions. The SSC criterion is based on comparing the current pressure in the system (grid cell) with the MCP for the given $\gamma$. If the current pressure in the grid cell is greater than the MCP, variable substitution from $(p, L, \gamma)$ to $(p, z)$ is performed. If the mixture in the grid cell forms a super-critical fluid, a negative-flash procedure is performed in order to obtain the MCP for the given $z$. The uniqueness of this switching criterion follows from the uniqueness of the critical tie-line and the MCP for a given $z$, or $\gamma$ (Iranshahr et al., 2009). The variable-substitution algorithm is schematically shown in Figure 2.14
2.4 Framework for general-purpose compositional simulation

The key aspects of our approach are (1) parametrization of the sub-critical space using a unique parameter associated with a tie-line, and (2) interpolation in the parameterized space. The framework is shown in Figure 2.15.
Figure 2.15: Framework for general-purpose compositional simulation
Chapter 3

Simulation Results

Simulation results using our Gamma Variable approach are compared with conventional EoS-based computations using the Natural and Molar Variables. The behavior of the different formulations is compared using four-, five- and eight-component systems. For each of these systems, immiscible and miscible gas displacement are investigated. A brief description of each system is given below.

1. System 1 (four-component system). The initial oil is made up of \(\{C_1(20\%), CO_2(1\%), C_4(29\%), C_{10}(50\%)\}\) at an initial pressure of 75 bars (above the bubble point). The injection gas is a mixture of two components \(\{CO_2(90\%), C_1(10\%)\}\). 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, and that 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 
\( \{C_1(20\%), \ CO_2(1\%), \ C_4(19\%), \ C_6(40\%), \ C_{15}(20\%)\} \) 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 \( \{CO_2(80\%), \ C_1(20\%)\} \). The injection pressure is 120 bars, which is lower than MMP for the system.

*Miscible case:* The injection composition is a mixture of four components 
\( \{C_1(8\%), \ CO_2(80\%), \ C_4(10\%), \ C_{15}(2\%)\} \); the injection pressure is 200 bars (above MMP).

3. System 3 (eight-component system). The initial oil is a mixture of 
\( \{C_1(10\%), \ CO_2(1\%), \ C_2(1\%), \ C_3(1\%), \ C_4(10\%), \ C_6(10\%), \ C_8(20\%), \ C_{15}(47\%)\} \) at a 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 \( \{CO_2(80\%), \ C_1(20\%)\} \). 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 a model is [60x220x1]. Other parameters are defined as follows: the size of a gridblock is 20x1x20 meters, the relative permeabilities are Corey functions with gas and oil exponents equal to two, and the rock compressibility is \( c_r = 7 \times 10^{-5} \ 1/\text{bar} \).
CHAPTER 3. SIMULATION RESULTS

3.1 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 parametrization using simplexes of different sizes are compared with conventional EoS based approaches. The size of a simplex is defined as the maximum distance between two supporting points in the simplex, i.e., \( L_\gamma = \| \gamma_i^* - \gamma_j^* \|_\infty \). 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 3.1: Distribution of log-permeability for upper layer of SPE 10 model

Figure 3.2 shows three different tessellations used for the convergence study; the sizes of the simplexes vary from very large \( (L_\gamma = 0.7) \), Figure 3.2 (a) to relatively small \( (L_\gamma = 0.021) \), Figure 3.2 (c). The results obtained with these tessellations and conventional EoS are compared in Figure 3.3. As expected, the highest interpolation error \( \approx 20\% \) is observed for the case with \( L_\gamma = 0.7 \); it should be mentioned, however, that this high error occurs around displacement fronts only. For the case of a very refined octree with \( L_\gamma = 0.021 \), excellent agreement of the results is observed; moreover, Figure 3.3 indicates that the interpolation error decreases linearly with
CHAPTER 3. SIMULATION RESULTS

simplex size. All these observations confirms convergence of the simulation results with tessellation refinement.

3.2 Numerical examples

3.2.1 Immiscible gas injection

Immiscible gas injection is modeled by employing 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.

- System 1 (four components): Figure 3.4 (a) shows the saturation distribution after 2000 days of gas injection; the difference in gas saturation (difference map) is shown in Figure 3.4 (b). These figures indicate 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 one that an IMPES approach would be able to take. The corresponding tessellated $\Gamma$-space is shown in Figure 3.5; 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 are presented in Figure 3.7. It can be seen that the Gamma Variables formulation requires the least CPU time. This is, mainly, because of less stability testing compared with the Natural Variables formulations. The number of Newton iterations is summarized in Table 3.1. The Natural and Gamma variables formulations show similar numbers of nonlinear iteration; whereas, the Molar Variables simulation needs greater numbers of iterations, which leads to the greatest CPU time among three sets.

- System 2 (five components): The simulation results are presented in Figure 3.7 (average CFL $\approx 203$). Here, the Gamma Variables formulation consumes the
Figure 3.2: Tessellated $\Gamma$-space for the five component system: $L_\gamma = 0.7$ (a), $L_\gamma = 0.176$ (b) and $L_\gamma = 0.021$ (c). Red dots are the supporting tie-lines. Green dots are the interpolated tie-lines.
Figure 3.3: Difference in gas saturation between the *Gamma* and *Natural* variables formulations after 2000 days of simulation: $L_\gamma = 0.7$ (a), $L_\gamma = 0.176$ (b) and $L_\gamma = 0.021$ (c)
least CPU time. Again, the *Molar Variables* formulation shows both the longest simulation time and largest number of Newton iterations (Table 3.1).

- System 3 (eight components): Figure 3.6 (a) and (b) show the saturation distribution and the difference map after 3000 days of gas injection. These figures indicate good agreement between the Gamma- and conventional EoS-based approaches. The tessellated Γ-space cannot be shown here because the dimension of the space is higher than three; 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 the Systems 1 and 2) conclusions about the performance of different nonlinear formulations are applicable here: the *Gamma Variables* formulation provides the least CPU time and is competitive with the *Natural Variables* formulation (see 3.9 and Table 3.1).

Table 3.1: Performance comparison (immiscible gas injection) between different nonlinear formulations. The number of wasted iterations is shown in parenthesis

<table>
<thead>
<tr>
<th></th>
<th>Natural Variables</th>
<th>Molar Variables</th>
<th>Gamma Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>System 1</td>
<td>280</td>
<td>303</td>
<td>279</td>
</tr>
<tr>
<td>System 2</td>
<td>401</td>
<td>405 (40)</td>
<td>383</td>
</tr>
<tr>
<td>System 3</td>
<td>455</td>
<td>491</td>
<td>456</td>
</tr>
</tbody>
</table>

### 3.2.2 Miscible gas injection

Miscible gas injection is modeled using Systems 1-3; in all of these systems, the injection pressure is higher than the Minimum Miscibility Pressure in order to achieve miscibility of the injected gas with the initial oil.

- System 1 (four components): Figure 3.10 (a) shows the saturation distribution after 2000 days of gas injection; the difference map is shown in Figure 3.10 (b).
Figure 3.4: Distribution of gas saturation (System 1, immiscible displacement) after 2000 days of simulation (a) and the difference in saturation for the Gamma and Natural variables formulations (b).
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Figure 3.5: Tessellated \( \Gamma \)-space – System 1.

The average CFL number is 465. These figures show good agreement between the Gamma and Natural variables formulations.

As opposed to the immiscible gas injection cases, the Natural Variables formulation shows the greatest number of Newton iterations (Table 3.2) and the longest CPU time (Figure 3.13). 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): Simulation results and the difference map are presented in Figures 3.11 (a) and (b), respectively (average CFL \( \approx 392 \)). Similar to the four-component example, the largest interpolation error is observed around miscible fronts (\( \approx 7\% \)).

The performance results are presented in Figure 3.14 and Table 3.2. Here, again, the Gamma Variables formulation provides 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): Figures 3.12 (a) and (b) show the gas saturation
Figure 3.6: Distribution of gas saturation (System 3, immiscible displacement) after 3000 days of simulation (a) and the difference in saturation for the Gamma and Natural variables formulations (b).
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Figure 3.7: Performance comparison for different nonlinear formulations – System 1 (immiscible displacement)

Figure 3.8: Performance comparison for different nonlinear formulations – System 2 (immiscible displacement)
distribution and the difference in gas saturation after 2000 days. These figures indicate good agreement in the simulation results obtained with the Gamma and Natural variables.

Figure 3.15 and Table 3.2 show 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 least CPU time.
Figure 3.10: Distribution of gas saturation (System 1, miscible displacement) after 2000 days of simulation (a) and the difference in saturation for the Gamma and Natural variables formulations (b).
Figure 3.11: Distribution of gas saturation (System 2, miscible displacement) after 2000 days of simulation (a) and the difference in saturation for the Gamma and Natural variables formulations (b).
Figure 3.12: Distribution of gas saturation (System3, miscible displacement) after 2000 days of simulation (a) and the difference in saturation for the Gamma and Natural variables formulations (b).
Figure 3.13: Performance comparison for different nonlinear formulations – System 1 (miscible displacement)

Figure 3.14: Performance comparison for different nonlinear formulations – System 2 (miscible displacement)
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Figure 3.15: Performance comparison for different nonlinear formulations – System 3 (miscible displacement)

Table 3.2: Performance comparison (miscible gas injection) between different nonlinear formulations. The number of wasted iterations is shown in parenthesis.

<table>
<thead>
<tr>
<th>System</th>
<th>Natural Variables</th>
<th>Molar Variables</th>
<th>Gamma Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>System 1</td>
<td>783(140)</td>
<td>364</td>
<td>381</td>
</tr>
<tr>
<td>System 2</td>
<td>806(260)</td>
<td>333(20)</td>
<td>422</td>
</tr>
<tr>
<td>System 3</td>
<td>630(200)</td>
<td>400(20)</td>
<td>377</td>
</tr>
</tbody>
</table>
Chapter 4

Conclusions

A new approach based on adaptive compositional space parameterization (ACSP) is proposed for numerical compositional flow simulation. The methodology builds on previous works on tie-line (more generally, tie-simplex) based parameterization (Voskov and Tchelepi, 2009c,b, 2008). The power of the proposed approach comes from the fact that a discrete representation of the $\Gamma$–space is capable of representing the thermodynamic phase behavior, and that the solution path associated with compositional displacements is nearly invariant with respect to changes in the hydrodynamic properties.

In this work, the applicability of the ACSP method is shown. The efficiency of the approach is based on adaptive interpolation of phase compositions using information from the discretized tie-line space. The tie-line space is discretized by a special technique, which is based on the generalization of the octree data structure. This allows us to overcome issues related to the dimension of the tie-line space. Moreover, by using this technique the desired regularity of the tessellation simplexes is guaranteed. Another advantage of the ACSP approach is accurate representation of the near-critical region and robust variable switching criteria for the representation of the super-critical region.

The ACSP- and EOS-based methods have been compared for both immiscible and miscible gas injections problems. The accuracy of the ACSP method is demonstrated, even when a small number of simplexes is used to discretized the compositional space.
The ACSP approach is quite stable; as a result, the computations are free of oscillations, and the accuracy can be controlled to arbitrary levels by refining the $\Gamma$–space discretization.

In terms of computational efficiency, the ACSP method reduces the cost of the thermodynamic equilibrium computations substantially compared with the standard EOS- based approaches. In terms of nonlinear behavior, it is shown that the Gamma Variables formulation takes advantages of the Natural Variables formulation for modeling of immiscible displacements and the Molar Variables formulation for modeling miscible gas injection problems.

While further development and testing are needed, the method can be seen as a Gamma Variables formulation for general-purpose compositional simulation. There are different possibilities to improve the framework: modification of the nonlinear solver based on the properties of solution path in the $\Gamma$-space, improved linear solver based on the decoupling of the elliptic (pressure) and hyperbolic ($\gamma$) variables, and new CFL criteria for adaptive implicit schemes, are not a complete list of a possible research directions.
Nomenclature

\( \gamma \)  Tie-line parameter

\( \gamma_k^* \)  Coordinates of \( k^{th} \) supporting point

\( \lambda \)  Simplex barycentric coordinates

\( k \)  Absolute permeability tensor

\( x_k^* \)  Phase compositions associated with \( k^{th} \) supporting point

\( \mu_j \)  Viscosity of phase \( j \)

\( \phi \)  Porosity

\( \Phi_i \)  Fugacity coefficient of component \( i \)

\( \rho_j \)  Molar density of phase \( j \)

\( f_{i,j} \)  Fugacity of component \( i \) in phase \( j \)

\( K_i \)  Equilibrium ratio of component \( i \) (\( K \)-value)

\( k_{rj} \)  Relative permeability of phase \( j \)

\( L \)  Liquid phase fraction

\( n_c \)  Number of components

\( p \)  Pressure

\( p_{ci} \)  Critical pressure for component \( i \)
CHAPTER 4. CONCLUSIONS

\begin{align*}
S_j & \quad \text{Saturation of phase } j \\
T & \quad \text{Temperature} \\
T_{ci} & \quad \text{Critical temperature for component } i \\
w_i & \quad \text{Acentric factor for component } i \\
x_{i,j} & \quad \text{Mole fraction of component } i \text{ in phase } j \\
z_i & \quad \text{Overall composition of component } i
\end{align*}
Bibliography


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