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Multiscale reconstruction in physics for compositional simulation

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ABSTRACT

A compositional formulation is a reliable option for understanding the complex subsurface processes and the associated physical changes. However, this type of model has a great computational cost, since the number of equations that needs to be solved in each grid block increases proportionally with the number of components employed. To address this issue, we herewith propose a multiscale reconstruction in physics for compositional simulation. The ideology consists of two stages, wherein two different sets of restriction and prolongation operators are defined based on the dynamics of compositional transport. In the first stage, an operator restricting the arbitrary number of components to only two equations for flow and transport is implemented with the objective of accurately reconstructing the multiphase boundaries in space. The prediction of multiphase front propagation is the most critical aspect of the approach, as they involve a lot of uncertainties. Once the position of two-phase boundaries is identified, the full conservative solution in the single-phase region can be accurately reconstructed based on the prolongation interpolation operator. Subsequently, in the second stage, the solution for the multicomponent problem (full system) in the two-phase region is reconstructed by solving just two transport equations with the aid of restriction operator defined based on an invariant thermodynamic path. The proposed reconstruction strategy results in coarsening of the compositional problem in terms of the physical representation (number of equations), thereby appreciably reducing the simulation time by several folds without significant loss in the accuracy. We demonstrate the applicability of the proposed multiscale strategy for several challenging gas injection problems.

1. Introduction

A compositional model is an inevitable and important tool in understanding the subsurface processes. The solution for this multi-component multiphase flow problem is determined by solving the associated nonlinear governing equations [1]. An equations of state (EoS) model is generally employed to describe the phase behavior of the system, and they are in turn resolved in two stages: phase stability test [2] and flash calculation [3]. A nonlinear system of thermodynamic constraints is used to represent the instantaneous thermodynamic equilibrium of the mixture. The aforesaid procedure is generally referred to as the standard EoS based approach for solving compositional problem [4]. On the other hand, these simulations

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are computationally intensive and demanding since the number of equations that needs to be solved in each grid block and in each iteration is remarkably high.

One possibility to improve the performance of reservoir simulation is to apply a multi-scale approach. It helps to reconstruct a fine-scale solution close to the cost of a coarse-scale solution with the controlled error in accuracy, thereby making it an attractive proxy model. Various multi-scale methods have been developed for the application of reservoir simulation [5–7]. Amongst them, Multi-Scale Finite Volume methods have become a state of the art in modern reservoir simulation [8–10], as they improved the performance by several folds. But most of the multi-scale methods are limited to the elliptic solution (global pressure or conductive temperature), without improving the hyperbolic part (saturation or composition). The only exception is the work by [11], where they used different operators for saturation reconstruction in the heuristic-driven front tracking and, [12], where they used an adaptive mesh refinement based on an algebraic multi-scale.

Significant progress has been made in the past to enhance the performance of compositional simulators. Specifically, several efforts were made to describe the entire system on the basis of pseudo-ternary representation [13,14]. Such representations were found to be valid for general compositional problem [15]. It was also shown that the solution route enters and exits the two-phase region by a shock and that these shocks coincide with the tie-line and its extension [15]. Later, an insightful demonstration on the basis of a unified Method of Characteristics (MOC) framework was carried out on a gas injection processes [16,17]. The theory was limited to a dispersion-free 1D displacement problem and it was shown that the entire displacement path can be constructed based on the key tie-lines of the system. It was also proven that the structure and properties of the tie-line dictate the solution route in the compositional space [18].

Based on these insights, a general approach for solving a compositional problem with the assumption of constant partitioning coefficients was proposed in [19]. This approach used the fact that the structure of the solution in tie-line space is independent of changes in hydrodynamic properties of the system. However, this fact was based on a general key tie-line theory and was not appropriately proven. A numerical framework describing similar ideology (based on the tie-line concept) was later implemented on more general case [20], where the original compositional problem was projected onto a tie-line space, and later, the parameters pertaining to a two-phase region of EoS based system are determined by polynomial approximations.

Subsequently, further developments were made in determining the solution of the compositional problem in the tie-line space. One approach was the use of multi-linear interpolation techniques to represent the thermodynamic phase behavior of the system which was referred to as the Compositional Space Parameterization (CSP) [21]. Also, it was proven that the projection of the solution to the tie-line space is invariant to the hydrodynamic parameters of the problem [22]. The CSP ideology eventually led to the development of Compositional Space Adaptive Tabulation (CSAT) method [21], where the tie-lines are stored in a table and later looked up to obtain the phase state of the mixture. The key to CSAT implementation is based on the fact that the phase state identification in a gas injection processes involves only a limited number of tie-lines. The proposed techniques not only accelerated the phase behavior computations, but also provided the basis for the development of fully EOS-free compositional simulation approach [23].

Another way to reduce the computational burden of compositional simulation is to reduce the number of equations solved per control volume. The most straightforward way is by adopting an Implicit Pressure Explicit Composition (IMPEC) reduction [24,25]. In this approach, the only global equation that needs to be solved in each grid-block is the pressure equation. The framework is constructed using an IMPEC reduction of full conservation equations with explicitly approximated composition. While this approach helps to reduce the number of global equations, it introduces a severe restriction to the computational time step due to the explicit treatment of hyperbolic variables [26].

This limitation can be overcome by applying Adaptive Implicit Method (AIM) [27,28]. In this method, the IMPES reduction is applied to only those grid cells where Courant–Friedrich–Lewy (CFL) condition [29] is below one, and thereby removing the time step restriction of the IMPES method. The AIM approach can significantly reduce the number of equations, in the case when a significant number of control-volumes stays close to the original state [30]. However, the AIM approach introduces an error at the interface between explicit and implicit block which can affect nonlinear convergence [31]. In addition, the AIM stategy strongly relies on natural variables formulation.

In this work, we propose a multiscale strategy for the solution of a compositional problem using molar formulation with significant changes in composition. We introduce two different sets of multiscale operators based on the dynamics of the hyperbolic problem. Initially, a fine scale restriction operator based on MOC theory [18] is applied to reduce the number of conservation equations to a single transport equation, which helps to reconstruct boundaries of the two-phase region. Once these boundaries are identified, the full solution in single-phase regions is reconstructed using an interpolation-based prolongation operator. Next, the solution for the full compositional problem in the two-phase region is reconstructed by solving just two transport equations with restriction and prolongation operators based on Compositional Space Parameterization technique.

The paper is organized as follows: a brief overview of the standard EOS based simulation approach is described first. Then the methodology and framework pertaining to the multiscale reconstruction strategy of a compositional problem are explained. Later, their application to multicomponent gas injection problems (including vaporizing and condensing gas drives) along with the supporting results are discussed. The conclusion and scope for further developments are given in the last section.

2. Conventional compositional approach

The solution framework for the compositional problem can be broadly separated into two sections, namely the thermodynamic part and the hydrodynamic part.

2.1. Hydrodynamic model

The hydrodynamic framework attributes to the solution of flow and transport equations, thereby determining the pressure (p) and the compositional changes (z) of the system. For an isothermal compositional system consisting of n_c components and two hydrocarbon phases (vapor and liquid) [23], the conservation equations of molar mass can be written as

$$\frac{\partial}{\partial t}\phi\left[(x_i\rho_o S_o)+(y_i\rho_g S_g)\right]+\nabla\cdot\left[(x_i\overline{u_o}\rho_o)+(y_i\overline{u_g}\rho_g)\right]+\left[(x_i\rho_o q_o)+(y_i\rho_g q_g)\right]=0,\ \ i=1,\ldots,n_c. \tag{1}$$

The velocity of the fluid phase, neglecting gravity and capillarity, is described based on Darcy's law as

$$\overline{u_j}=-\overline{\overline{K}}\frac{k_{rj}}{\mu_j}\nabla p,\quad j=1,2. \tag{2}$$

For a 1D incompressible isothermal problem, the governing mass conservation equation can be simplified [21] as shown in

$$\frac{\partial z_i}{\partial t}+\frac{u_t}{\phi}\frac{\partial F_i}{\partial x}=0,\quad i=1,\ldots,n_c. \tag{3}$$

We will be using this form for simplicity of description without limiting a general applicability of the proposed technique. Here z_i is defined as

$$z_i=\frac{x_i\rho_o S_o+y_i\rho_g S_g}{\rho_o S_o+\rho_g S_g}, \tag{4}$$

and can be found from the vapor fraction

$$v=\frac{\rho_g S_g}{\rho_o S_o+\rho_g S_g}, \tag{5}$$

$$z_i=x_i(1-v)+y_i v. \tag{6}$$

The 'F_i' is further expanded based on the linear relationship as shown,

$$F_i=x_i(1-f_g)+y_i f_g,\qquad i=1,\ldots,(n_c-1). \tag{7}$$

Finally, the auxiliary relations used in closing the system of equations are given by

$$\sum_{i=1}^{n_c}x_i=1\quad\&\quad\sum_{i=1}^{n_c}y_i=1, \tag{8}$$

$$S_o+S_g=1. \tag{9}$$

2.2. Thermodynamic model

The thermodynamic framework enables us to determine the phase behavior of the system with the aid of phase stability test [2] – to identify the number of phase in a particular grid cell and flash calculation [3] – to determine the split fraction of components amongst the phases present. The flash calculation can be carried out either based on equilibrium ratios (also known as K values) or based on equations of state (EoS). In this research work, we have followed the K-value based methodology to perform flash calculations. This assumption does not limit the applicability of the proposed technique to a general EoS-based system.

In a K-value based system, the general phase split procedure is reduced to the solution of the following equation:

$$h(v)=\sum_{i=1}^{n_c}\left[\frac{z_i(K_i-1)}{v(K_i-1)+1}\right]=0. \tag{10}$$

The nonlinear equ. (10) is also referred as the Rachford–Rice equation [32], which can be solved by a combination of bisection and Newton's method to determine the vapor phase fraction (v). It is also worth noticing that the concept of flash calculation is not limited to two-phase mixtures alone as they can also be performed on single-phase compositions [32,33].

Such a phase computation is generally referred to as the negative-flash calculation, where the equ. (10) is solved for the vapor phase fraction (v) of single-phase compositions. The idea behind the negative flash calculation is that a single-phase mixture is present as a linear combination of phase composition and it always lies on the extension of the tie-lines. In this study, we have adopted the negative flash based framework to determine the phase behavior of the system.

In order to close the system of equations, additional constraints between the components and the phases exist under the statement of instantaneous thermodynamic equilibrium – which is in turn expressed as equality in fugacity of the vapor and liquid phases [34], refer equ. (11) below

$$f_{i,g}(p, T, y_i) = f_{i,o}(p, T, x_i). \tag{11}$$

The fugacity is a function of pressure (p), temperature (T) and the phase compositions ($x_{i,j}$) and it is generally determined based on the equations of state (EoS).

A sequential framework, explicit in time, is used in solving the system of equations equ. (3), (9) with various closing relations, thereby determining the solution for the unknown variables (1 pressure, two-phase saturations and $n_c \times n_p$ phase compositions) in each grid block.

3. Multiscale reconstruction in physics

In order to gain better insight into the proposed multiscale technique, the basics pertaining to the construction of solution is initially discussed. In a compositional formulation, the physical system is represented as a mixture of different components with different volume fractions. For instance, in a 3-component system, these mixtures are referred to as the light, intermediate and heavy hydrocarbon component. At given thermodynamic conditions (pressure and temperature), the light component is present in a gas phase and the heavy component is present in a liquid phase. The intermediate component is generally present in either of these two phases (liquid or gas). The phase behavior of such systems (at a fixed pressure and temperature) is directly driven by the compositional changes and it is generally represented on a phase diagram. Fig. 1 shows the phase diagram, the fractional flow curve and the compositional profile of light component for a ternary gas injection process.

The dew point and bubble point curves (blue and green line in Fig. 1(a)), which are collectively referred as the binodal curve, distinguish the single-phase compositions with those existing in two phases. The two-phase compositions lie inside of the binodal curve and they are further split into liquid and vapor phase fraction. These phase fractions inside the two-phase region are eventually connected by a *tie-line* (black dotted line in Fig. 1(a)). Both the binodal curve and the equilibrium tie-lines are strong functions of pressure and temperature with weak dependency on composition.

Further, the trajectory (or path) that describes the compositional changes between the initial oil composition and the injected gas composition is referred to as the *compositional path*. The salient principles that govern the construction of the solution (compositional path) are the *conservation* and *entropy* conditions, resulting in a series of self-sharpening waves (shocks) and spreading waves (rarefaction) as shown in Fig. 1. These changes are generally consistent with the above described physical principles.

The fractional flow theory gives insight on the fluid mobility in the presence of other fluid phases. Fig. 1(b) shows the plot of fractional flow as a function of composition. The two curves, shown in the plot, refer to fractional flow on the injection (red curve) and initial tie-line (blue curve) for a three-component system, and the construction of solution path is subsequently explained. The velocity (a.k.a. slope of the fractional flow curve) of each composition follows a simple rule where the characteristic velocity should monotonically increase from injection to initial composition. This corresponds to the fact that in the stable solution, the slower waves cannot propogate ahead of the faster waves. If the slower waves from compositions close to the initial conditions originate ahead of faster waves, a shock will form as the faster waves overtake the slower waves. Hence, by satisfying this condition, the consistent solution contains two shocks connecting initial and injection compositions and it is generally independent of the number of components present in the system [16,17]. These two shocks are referred to as the *leading* and *trailing shocks*.

From a physical perspective, the leading shock is formed because of the rapid movement of the injected fluid when compared with the initial oil composition, and the trailing shock is formed due to evaporation of the intermediate components into the unsaturated injected fluid. The velocity of these two shocks depends on the injection and the initial compositions. Between these two shocks, the fan of characteristics associated with the continuous variation of composition forms, which is also known as the *spreading* or *rarefaction* waves [15]. This continuous variation in the compositions can occur along the tie-line (known as tie-line rarefaction path), and as well as between the tie-lines (known as non-tie-line rarefaction path), refer Fig. 1.

Further insight into the shock solution is described based on the Rankine–Hugoniot condition [15], which is given by the equ. (12):

$$\Lambda = \frac{dF_i}{dz_i} = \frac{F_{i,2} - F_{i,1}}{z_{i,2} - z_{i,1}} \quad i = 1, \ldots, n_c, \tag{12}$$

where, $F_{i,1}$ & $z_{i,1}$ represents the fractional flow and composition of component 'i' on the downstream side of the shock and $F_{i,2}$ & $z_{i,2}$ represents the fractional flow and composition of component 'i' on the upstream of the shock. The Rankine–

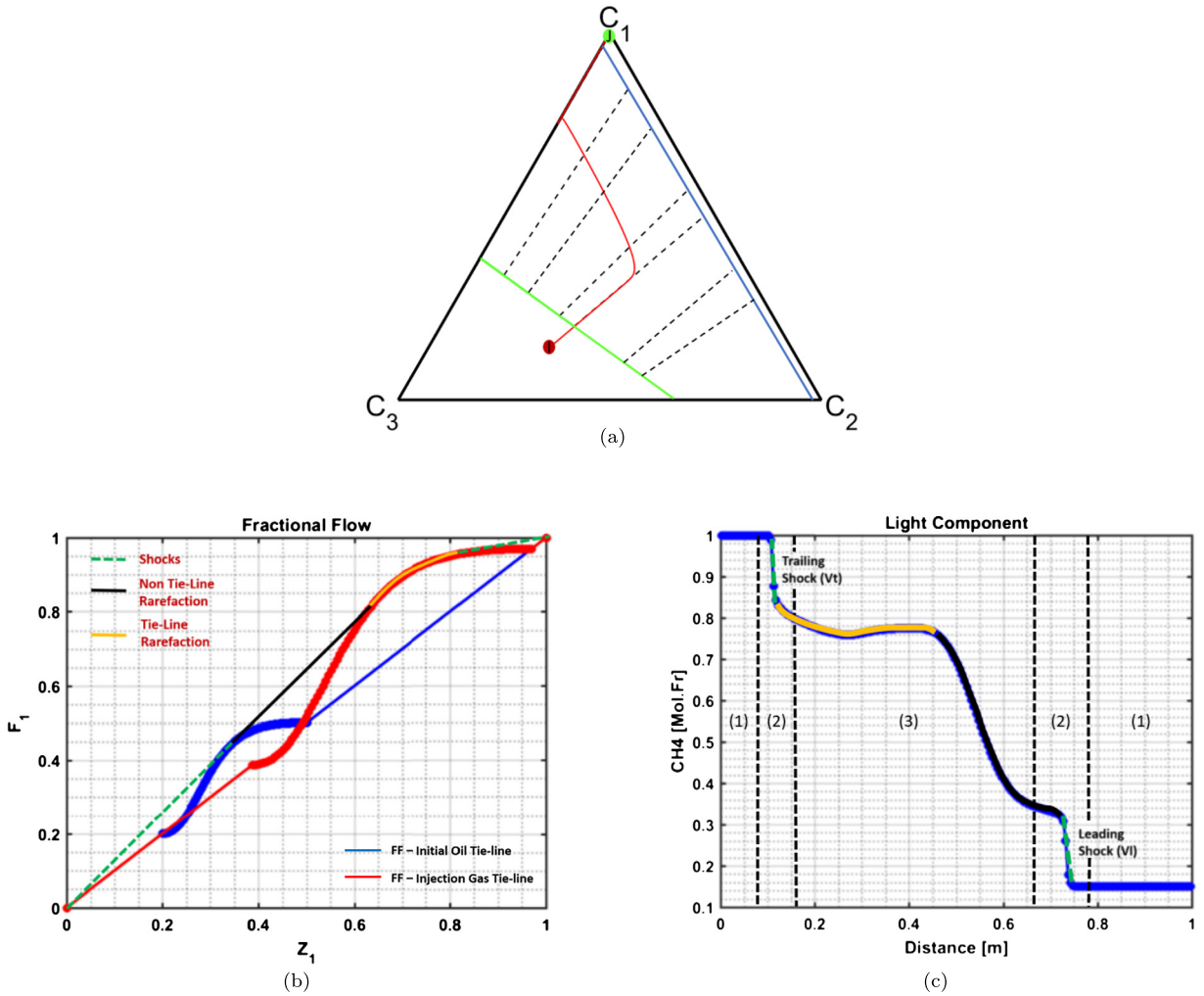


Fig. 1. General structure of compositional solution: (a) ternary phase diagram, (b) fractional flow curve and (c) solution profile (light component). (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

Hugoniot condition is an integral version of the conservation equation shown in equ. (3) and it illustrates the fact that the volume is conserved across the shock.

Now, the outset of multiscale based reconstruction technique is attributed to the saturation history (Fig. 1(c)) of the compositional problem, since the profile can be classified into three distinct regions based on the characteristic changes [11]. The region 1 corresponds to a placid zone, where the gas saturation value remains (almost) constant. The region 2 corresponds to shock solution, where there is a pronounced jump in the saturation values. The characteristics of this region are defined based on the Rankine–Hugoniot condition, see equ. (12). Finally, the region 3 refers to a fan characteristics (rarefactions), where the saturation changes are more continuous. The region 1 and region 3 are referred to as “single-phase region” and “two-phase region” respectively, while region 2 is a “transition zone”. On the basis of this classification, it can be observed that the shock separates two contrasting zones of saturation, with these zones located on either side of it. This apprehending fact forms the basis of the proposed multiscale technique, where specially constructed restriction and prolongation operators are implemented on the different regions of saturation to reconstruct the solution of the hyperbolic problem (full system).

Initially, we reconstruct the position of shock in space as they hold the key, and it is carried out using a fine scale restriction operator. Once the position of shocks is identified, the interpolation-based prolongation operator is applied for the reconstruction of the solution in single-phase regions similar to the approach suggested in [11]. Later, the solution for n_c components lying in between the leading and trailing shock is reconstructed with the aid of the restriction and prolongation operators defined based on CSP technique [21]. Both vaporizing and condensing gas drives (refer Table 1 & 2 for compositions) have been implemented based on the proposed approach and the corresponding results are discussed in the subsequent sections.

Table 1
Vaporizing gas drive.

Comp.	C1	CO2	C4	C10
Initial	0.10	0.18	0.37	0.35
Injection	0.97	0.01	0.01	0.01
K-value	2.5	1.5	0.5	0.05

Table 2
Condensing gas drive.

Comp.	C1	CO2	C4	C10
Initial	0.01	0.01	0.39	0.59
Injection	0.59	0.39	0.01	0.01
K-value	2.5	1.5	0.5	0.05

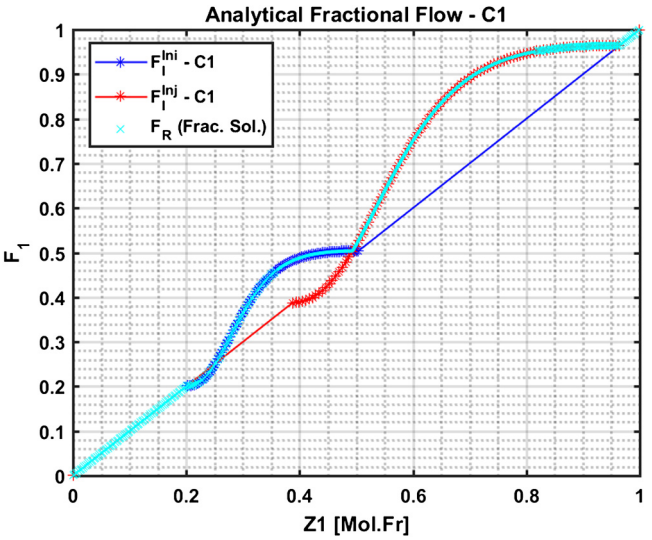


Fig. 2. Analytically constructed fractional flow curve for light component (CH_4) in a vaporizing gas drive.

4. Multiscale reconstruction of single-phase region

The tracking of front propagation for a compositional transport problem is carried out based on analytically constructed fractional flow curves, which in turn play the role of restriction operator. Initially, the liquid (x_i) and the vapor (y_i) fraction values of the compositions lying on the extension of injection and initial tie-lines (single-phase region) are selected from the negative flash calculation. Further, by keeping this x_i and y_i values constant, the fractional flow curve is analytically constructed in the two-phase region based on equ. (7) [20].

The fractional flow plot is an S-shaped curve within the two-phase region. In the single-phase region, the fractional flow value of a particular component varies linearly with the molar fraction of the corresponding component. Hence the fractional flow curve is just a straight line in the single-phase region (refer Fig. 1(a)). Two fractional flow curves for a chosen component I corresponding to initial and injection tie-line can be found from:

$$F_I^{ini} = x_I^{ini}(1 - f_g) + y_I^{ini} f_g, \quad F_I^{inj} = x_I^{inj}(1 - f_g) + y_I^{inj} f_g. \tag{13}$$

Once these curves are analytically constructed based on the key tie-lines of the system, they are eventually combined together, and an equivalent solution curve is constructed by taking a convex hull on the union of both curves:

$$F_R = \text{conv}(F_I^{inj} \cup F_I^{ini}). \tag{14}$$

This procedure results in a single analytic curve, that switches between the initial and injection fractional flow curve at the point of their intersection.

The analytically constructed curve shown in Fig. 2 represents the pseudo-fractional-flow curve for the reconstruction of leading and trailing shocks. Later, these values are tabulated and defined as restriction operator during the course of a simulation, thereby enabling us to accurately locate the shock positions in space. The simulation framework is analogous to a fully implicit solver except for the fact that the defined restriction operator is applied for the restricted transport equation:

$$\frac{\partial z_R}{\partial t} + \frac{u_t}{\phi}\frac{\partial F_R}{\partial x} = 0. \tag{15}$$

4.1. Application for 1D transport problem

Fig. 3 shows the reconstructed shock solution for a 4-component system (vaporizing gas drive). The results of the reconstructed solution are evaluated by comparing it with a reference full-physics solution. It can be observed that the shock

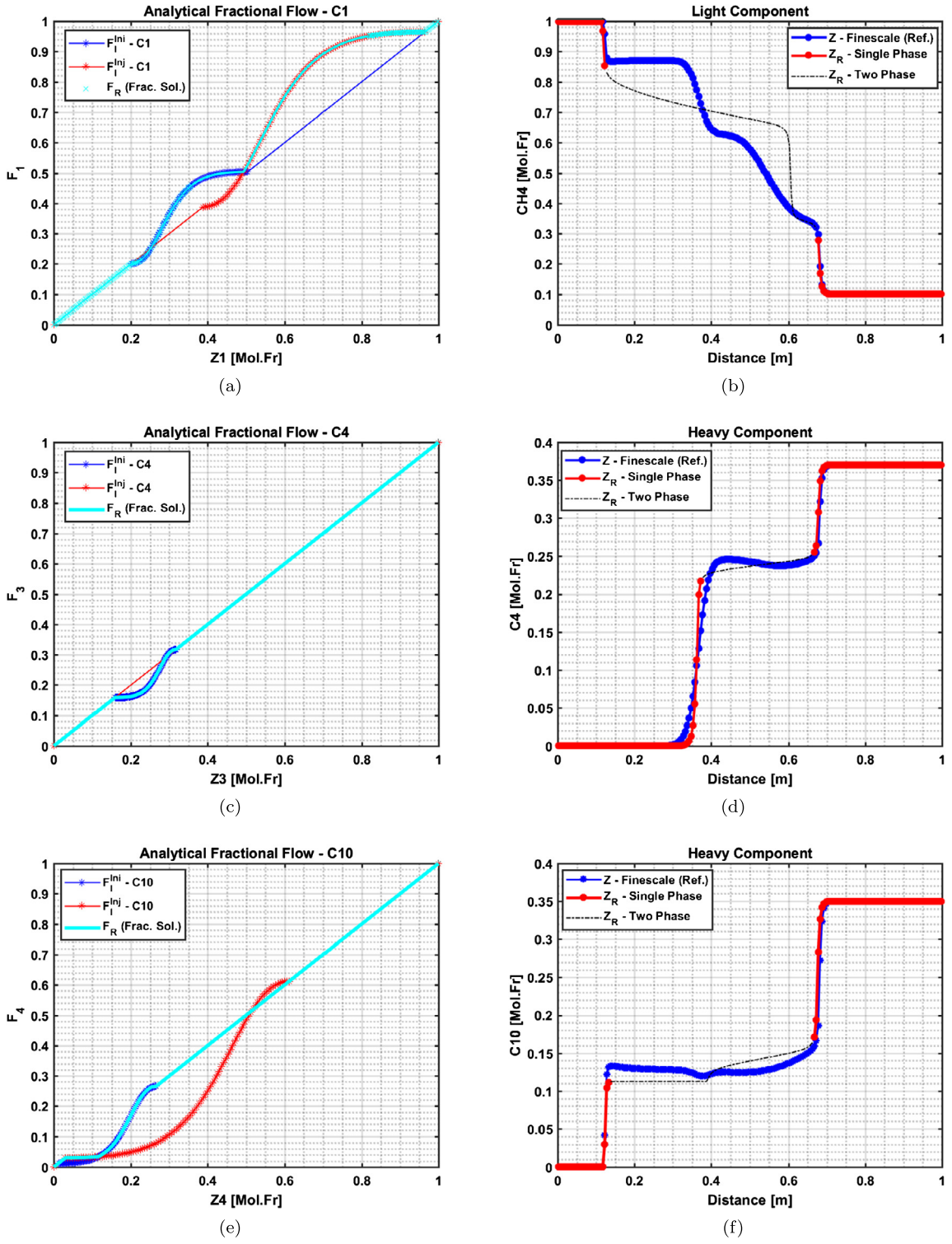


Fig. 3. Analytically constructed fractional flow curves (on left), and the corresponding reconstructed solution of transport problem (on right) for (a), (b) light component C_1, (c), (d) intermediate component C_4 and (e), (f) heavy component C_{10}.

positions are accurately reconstructed to fine-scale accuracy with the use of the restriction operator. On the other hand, the solution between the shocks (in the two-phase region) differs. Though there is a valid reason behind this mismatch (see discussion in Appendix A.2), this difference can be neglected since our objective is limited to the accuracy of shock recon-

struction. In this stage, our multiscale approach reduces the complexity (number of equations solved per control volume) from (n_c) conservation equations to two: [$n_c \times n_b \Rightarrow 2 \times n_b$], where n_b is the number of grid blocks and n_c is the number of components in the system. Further, the proposed methodology remains valid for any changes in the injection and initial streams. Under such circumstances, the negative flash calculation (equ. (10)) is performed on the new (injection/initial) composition, and equ. (13) – equ. (15) is eventually solved to determine the corresponding phase boundaries of the system.

Subsequently, the solution in the single-phase region is reconstructed using the prolongation operator based on interpolation of entire solution between injection and initial composition, and by using the concentration of pseudo-component from the solution of the restricted problem:

$$\boldsymbol{\kappa}(z_R)\left[\mathbb{R}^1 \Longrightarrow \mathbb{R}^{n_c-1}\right] : \mathbf{z} = \mathbf{I}_{\{z^{ini}, z^{inj}\}}(z_R). \tag{16}$$

Here, '$\boldsymbol{\kappa}$' is the interpolation-prolongation operator, 'z_R' is the reconstructed shock solution and '$\mathbf{I}$' is the piecewise linear interpolation function. This prolongation will match a conservative solution in single-phase regions due to the weak dependency between initial/injection compositions and compositions at shocks, controlled by Rankine–Hugoniot conditions shown in equ. (12). Notice that, conceptually this approach is similar to the prolongation operation for reconstruction of a fine-scale spatial solution proposed in [11].

4.2. Application for 2D transport problem

The proposed first stage reconstruction was also tested for flow and transport compositional problem in a highly heterogeneous reservoir. For this test, the top layer of SPE 10 model with heterogeneous porosity and permeability maps were used [35]. The model is built on a regular Cartesian grid (60 $\times$ 220 cells), with one gas injection well in the center and four production wells at corners. The implementation of the first stage reconstruction was carried out based on the OBL technique described in [36,37]. Here, we translate a constructed pseudo-fractional flow curve to convection operator and tabulate it as a function of nonlinear parameters (p and z_R). A pseudo-binary system is subsequently solved, thereby yielding the solution for pressure and indicator composition. Later, the solution for the full system (n_c components) is eventually reconstructed by linearly interpolating the full set of compositions between the initial and injection mixtures using the solution of indicator composition z_R. Once the full composition is reconstructed using (16), the negative flash procedure is applied to predict phase behavior and locate the boundaries of the multiphase region. In summary, irrespective of the size of the system, a pseudo binary model is sufficient enough to determine the phase boundaries for the corresponding full system.

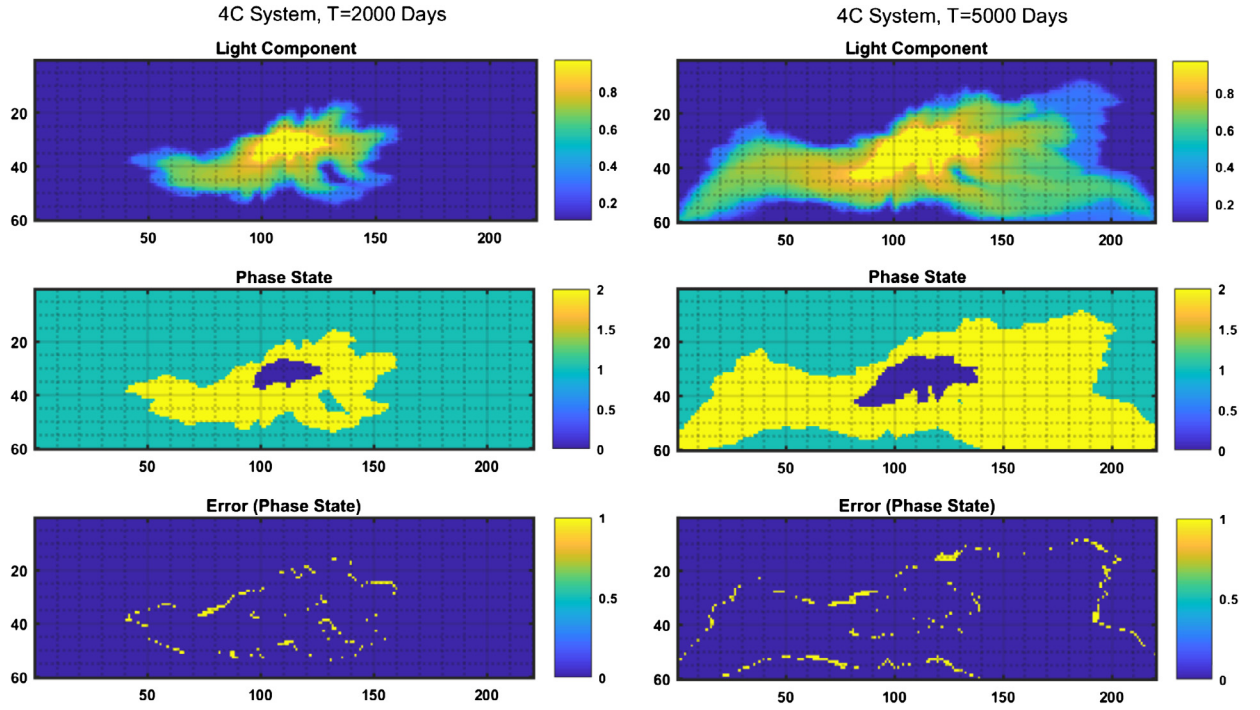
Fig. 4 shows the reconstructed shock solution of SPE 10 model at two different steps, for vaporizing gas drive system (main parameters are given in Table 5 and Fig. 10). The subplot in the figure shows the (1) compositional changes, (2) the phases state in each grid block and (3) the difference in phase state identification. The limited mismatch in phase boundaries between the full conventional approach and the proposed multi-scale reconstruction demonstrates the profoundness of the proposed first stage reconstruction.

5. Multiscale reconstruction of two-phase regions

The solution in the two-phase region is determined based on Compositional Space Parameterization technique [21]. The CSP approach was proposed to speed up the phase behavior calculations by replacing the flash calculation with interpolations in the parameter space of the problem. The phase behavior of gas-injection processes is predominantly controlled by the properties of two key tie-lines that extend through the initial and injection compositions, and hence it is convenient to parameterize the problem based on these two tie-lines. It has also been proven that the projection of compositional solutions with different hydrodynamic properties onto the tie-line space is invariant and only depends on thermodynamic properties of solution [22].

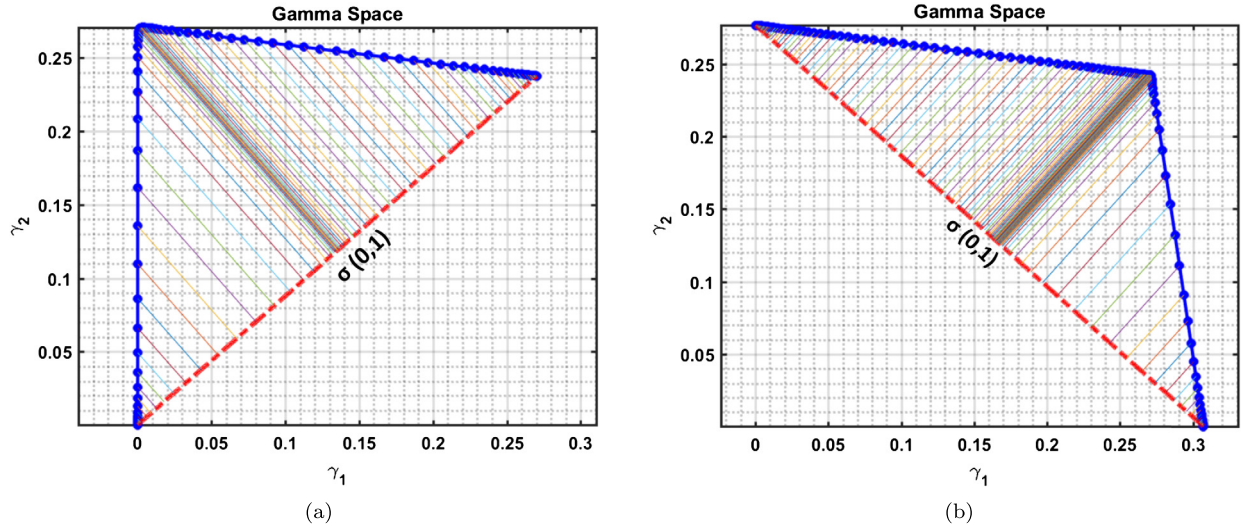
On the basis of parameterization technique, an advanced simulation framework has been proposed for the solution of a hydrodynamic problem, thereby reconstructing the solution in two-phase region [23]. This reconstruction is based on the invariance of a compositional solution in tie-line space. Notice that this technique requires either the solution of auxiliary thermodynamic problem [20], or the solution of a full problem and its projection onto the tie-line space [21]. Once constructed, this solution and its projection provide the basis for multiscale reconstruction independent of any changes in the hydrodynamic properties.

Initially, the existing tie-lines of the solution are parameterized based on '$\boldsymbol{\gamma}$' variables. By this, each tie-line in the system is uniquely identified. It is worth noticing that the parameterizing variables ($\boldsymbol{\gamma}$) can be defined arbitrarily in the compositional space, except for the fact that this definition should be unique. For instance, they can be defined as a tie-line trace on the face of compositional diagram [20], or at a plane representing the tie-line centers [21]. Also, the γ is constant along a tie-line, and changes only when the solution is switched between tie-lines. Once, the tie-lines are parameterized, the γ variable (vector quantity) is plotted on to a tie-line space (γ-space), and the resulting $\boldsymbol{\gamma}$-path present discontinuities (shocks and rarefactions) associated with the key tie-lines of the solution. In Fig. 5, the γ_1 and γ_2 refer to the phase fractions of intermediate components (CO2 & C4 for this case) in a four-component system introduced above.



(a) Solution after T=2000 days (b) Solution after T=5000 days

Fig. 4. First stage reconstruction in SPE-10 vaporizing gas drive for two different timesteps: (upper) composition of light component, (middle) phase identification and (lower) blocks with misidentified state.



(a) (b)

Fig. 5. Parameterized space (γ-path): (a) vaporizing gas drive and (b) condensing gas drive.

Once the Γ-path is constructed, a new variable 'σ' is introduced [38]. The objective of this 'σ' variable is to parameterize the γ-path and the same is accomplished by orthogonally projecting the 'γ' values onto 'σ' such that it ranges from 0 and 1 (Fig. 5). In this representation, all phase fractions become nonlinear with $y_i(\sigma)$ and $x_i(\sigma)$.

Following this procedure, the compositional variation of the entire problem is parameterized in tie-line space. Notice that this solution is invariant of changes in hydrodynamic properties of the problem and only dependent on thermodynamics and injection/initial conditions [20,22]. Now the solution for the two-phase region (area within the leading and trailing shocks) is determined by solving the transport problem in the parameterized space. First, we represent overall composition at new timestep through the nonlinear relation involving phase fractions:

$$z_i^{n+1} = y_i(\sigma^{n+1}) \cdot v^{n+1} + x_i(\sigma^{n+1}) \cdot (1 - v^{n+1}). \tag{17}$$

Now, we can substitute this relation into two conservation equations from (3) in discretized form. The resulting restricted system takes the following residual form:

$$R_i = y_i(\sigma^{n+1}) \cdot v^{n+1} + x_i(\sigma^{n+1}) \cdot (1 - v^{n+1}) - z^n - \frac{dt}{\phi \cdot dx} \{(F_i \cdot U_{i+1}) - (F_{i-1} \cdot U_i)\}^n \quad i = 1, 2. \tag{18}$$

Any two components can be arbitrarily chosen to solve equ. (18), here we select light and the heavy component. Further, an explicit flux approximation technique has been used to solve the non-linear system. Notice, that the type of flux approximation does not limit the application of the proposed approach. The equ. (18) is nonlinear in nature, even for an explicit flux approximation, and it is induced by the tie-line parameters (x_i and y_i). As a result, Newton's method has been applied to resolve the system and obtain the solution iteratively. Through this technique, the $n_c - 1$ transport equations of the original problem are replaced by just two equations depending on two variables only (σ and v). In other words, the equ. (18) is solved with parameterized variable σ and vapor fraction v as its primary unknowns instead of directly solving for the compositional changes (z_i), thereby resulting in the restriction of a full system. The final system of equations (in algebraic form) is given by equ. (19).

$$\begin{bmatrix} \frac{\partial R_1}{\partial \sigma} & \frac{\partial R_1}{\partial v} \\ \frac{\partial R_2}{\partial \sigma} & \frac{\partial R_2}{\partial v} \end{bmatrix} \begin{bmatrix} \delta\sigma \\ \delta v \end{bmatrix} = \begin{bmatrix} -R_1 \\ -R_2 \end{bmatrix}. \tag{19}$$

In the previous stage, the shock positions are located in space based on the solution with restriction operator and compositions in single-phase region are reconstructed using prolongation operator based on interpolation. Now, the solution lies in the two-phase region is restored by solving two restricted conservation equations (18) in the parameterized space.

Once the solution is obtained, the prolongation operator is applied again based on the projection of σ solution (points on the red curve) back to γ-path (points on the blue curve), see Fig. 5 for details. This operator can be expressed as

$$\boldsymbol{\psi}(v, \sigma) \left[\mathbb{R}^2 \Longrightarrow \mathbb{R}^{n_c - 1}\right] : \mathbf{z} = \mathbf{y}(\sigma) \cdot v + \mathbf{x}(\sigma) \cdot (1 - v). \tag{20}$$

Notice that γ-parameters uniquely identify tie-lines in the compositional space, which defines the corresponding values of **x** and **y**. Once tie-line is reconstructed based on σ, the corresponding overall compositions **z** are recovered using solution in 'v' and 'equ. (20)'.

Fig. 6 and Fig. 7 shows the solution of a vaporizing and condensing gas drive problem. It can be seen that the reconstructed two-phase region ('Z-CSP' curve) accurately matches with the reference fine scale solution. It is also worth noticing that the reconstructed solution of the entire compositional system is obtained by solving the restricted system (19) instead of the full set of conservation equations.

This makes the total cost of full multi-scale reconstruction $[n_b \times 2 + n_{b,2} \times 2]$ instead of $[n_b \times n_c]$, where n_b and $n_{b,2}$ correspond to the total number of blocks and the number of blocks in two-phase region respectively. On the whole, the cost of full reconstruction for n_c-component compositional solution becomes only slightly higher than the solution of the black-oil problem. Also, the decoupling between the thermodynamic and hydrodynamic problems provides a simpler platform to carry out a multi-dimensional analysis and sensitivity studies, since the Γ-path is independent of flow properties and only depends on thermodynamic parameters of the system.

Further, based on the description of the parameterization technique, it is also evident that the construction of γ-space is of paramount importance – which requires unique identification and parameterizing of the tie-lines involved in the conservative system. This, in turn, implies the fact that with any changes in the thermodynamics of the system (initial and injection compositions), the tie lines involved in the construction of conservative solution also changes, thereby resulting in a different γ-path. Fig. 8 shows the changes in the γ-path for a system with varying initial oil and injection gas compositions shown in Tables 3, 4. These compositional paths can be parameterized independently and used in the OBL framework [36, 37], thereby directly incorporating the compositional changes and thus making the proposed technique robust.

Also, the parameterization technique remains valid irrespective of the size of system, and it is enough to solve the same restricted system of equations with v and σ as primary unknowns. The only difference is in the dimension of the gamma-space, where invariant path is constructed. In other words, for a system of n_c components, the compositional space parameterization technique results in a tie-line space (γ-path) having $(n_c - 2)$ spatial dimensions [20]. For example, the Fig. 9 below shows the gamma path for a 5-component system and the corresponding results of reconstruction are shown in Appendix A.3.

6. Conclusion

Through this research work, a multiscale technique has been proposed to enhance the performance of compositional simulation. The methodology is based on the local compositional profile of the system and eventually, a two-stage reconstruction of the compositional problem is carried out. In this study, we present the application of the proposed approach for an idealized compositional problem with constant partition coefficients.

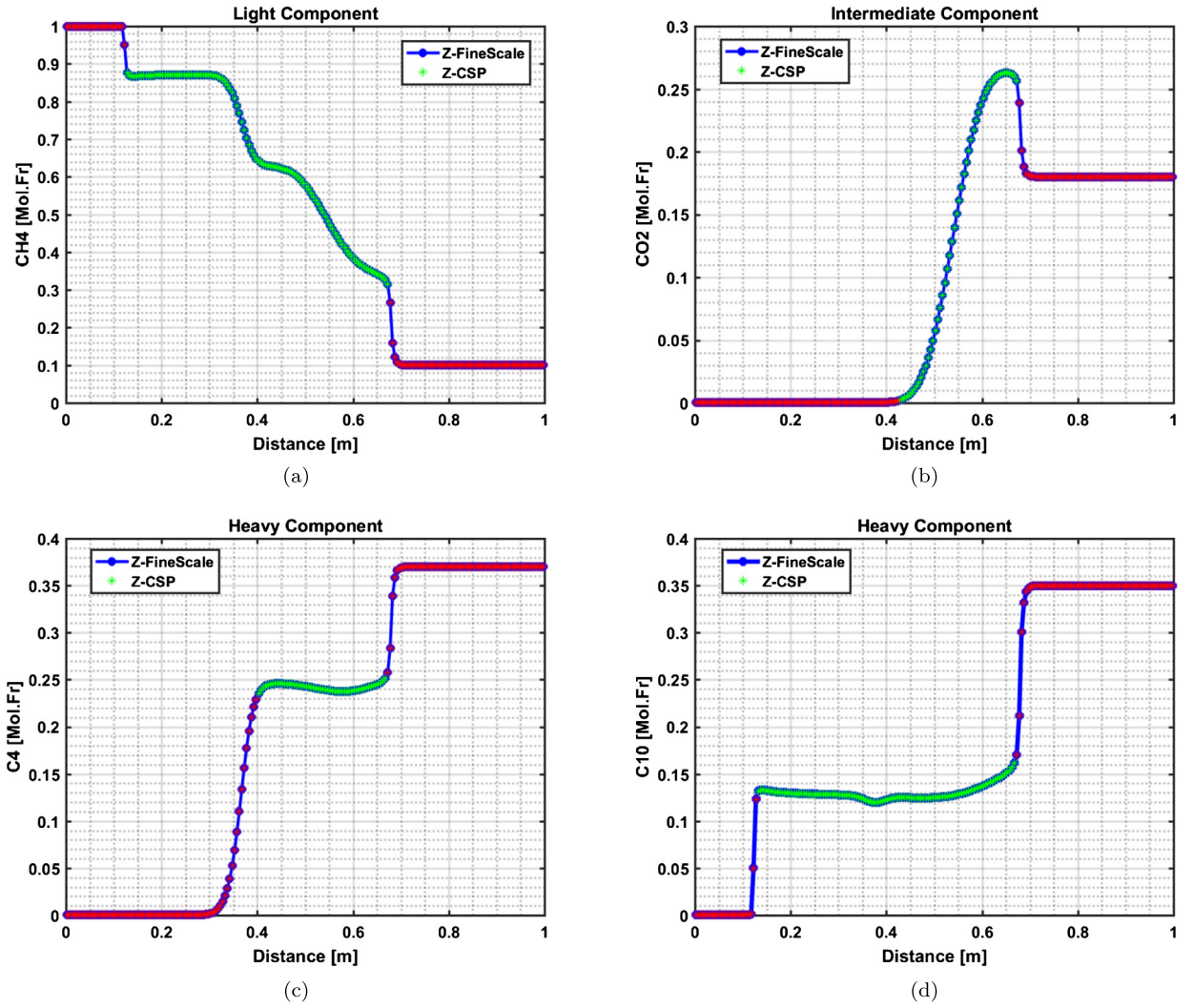


Fig. 6. Full reconstruction of four-component problem for vaporizing gas drive (a) light component CH_4 (b) first intermediate component CO_2 (c) second intermediate component C_4 (d) heavy component C_{10}.

First, we present the technique for predicting the front (shock) positions in space using the restriction operator based on fractional flow theory. The approach was tested for several 1D gas injection problems of practical interest, including the vaporizing and condensing gas drives, and it accurately predicts boundaries of the two-phase region. An interpolation-based prolongation operator was applied for the reconstruction of the single-phase region, thereby precisely matching the conservative solution of the full problem in this region. Subsequently, the approach was also extended to multidimensional problems with highly heterogeneous properties using Operator-Based Linearization (OBL) formalism.

The second stage of the proposed multiscale strategy is applied to reconstruct the compositional solution in the two-phase region. This reconstruction is performed using the restriction operator based on Compositional Space Parametrization (CSP) technique. The restriction operator reduces the full system of conservation equations to two equations per each control volume in the two-phase state. Based on the solution of this reduced system, a prolongation interpolation operator is applied in the tie-line space, which is capable of reconstructing a conservative fine scale solution of the full system.

While the proposed multiscale approach is found to be rewarding, there are several possibilities for its further improvements. The first and the foremost advancement would be to implement this technique in a fully implicit compositional framework involving complex nonlinear physics. The equations of state can also be directly incorporated for the phase behavior of the system. In addition, the approach could also be extended to problems with a strong initial compositional gradient or changes in injection/initial stream and the same can be archived by the direct application of OBL methodology. While the current implementation is limited to immiscible gas injection process, the extension of the methodology to near-miscible regimes is straightforward and is the focus of our current work. Finally, a similar approach can also be developed for thermal problems with an arbitrary number of phases.

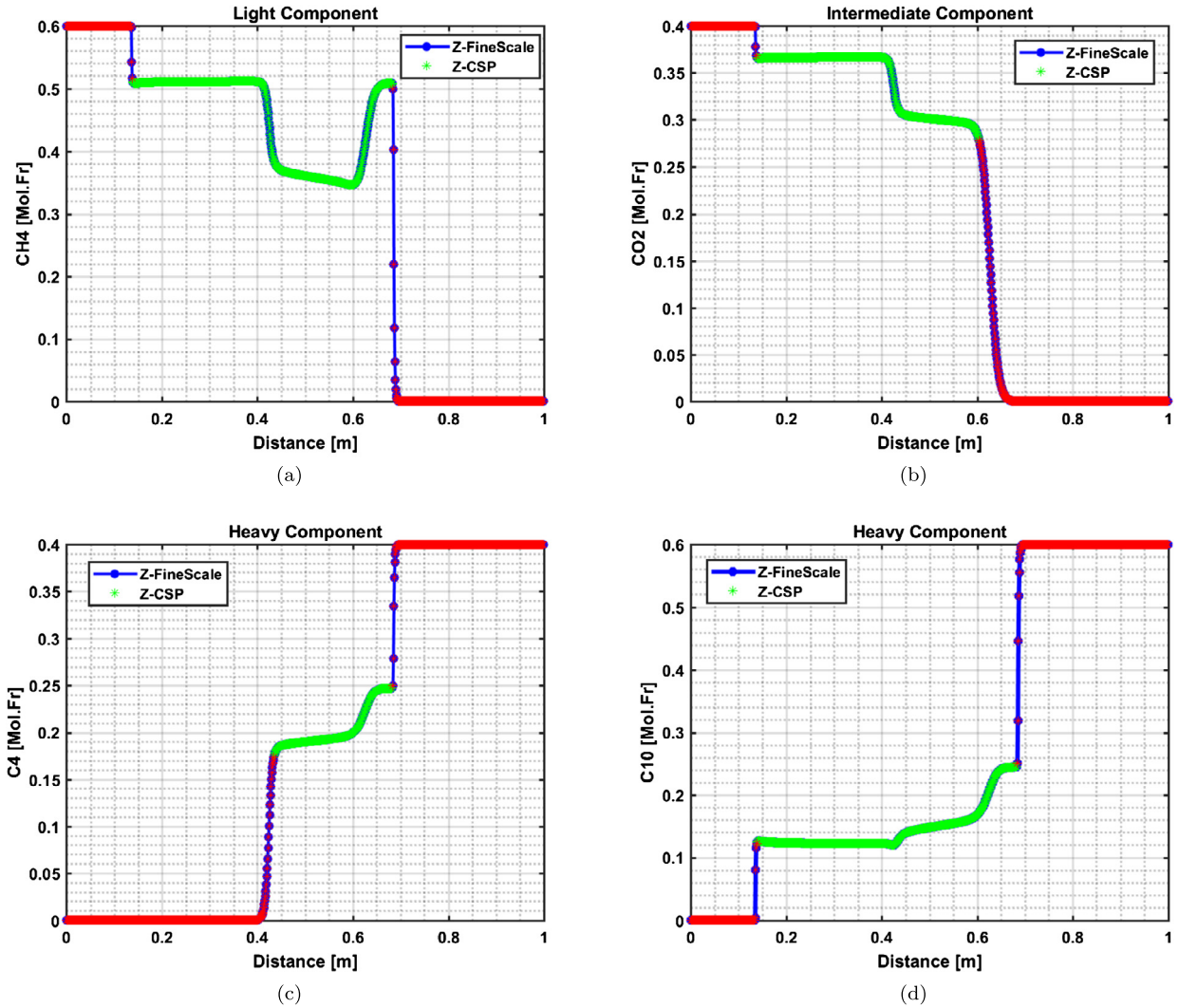


Fig. 7. Full reconstruction of four-component problem for condensing gas drive: (a) light component CH_4, (b) first intermediate component CO_2, (c) second intermediate component C_4 and (d) heavy component C_{10}.

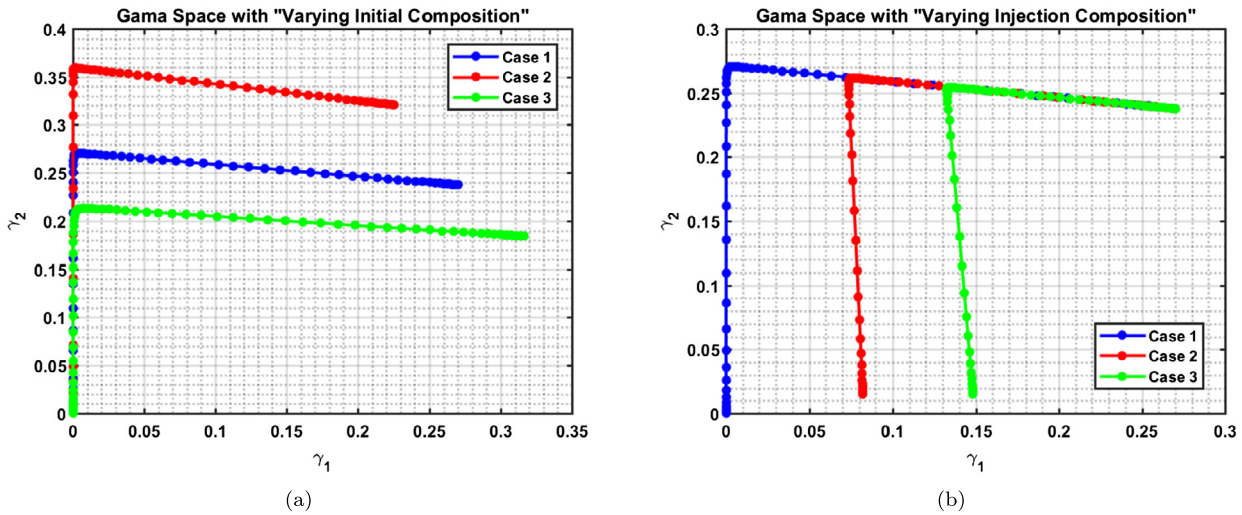


Fig. 8. Parameterized space (γ-path) for varying (a) initial oil and (b) injection gas compositions.

Table 3
Variations in initial oil composition.

Ini. comp.	C1	CO2	C4	C10
Case 1	0.10	0.18	0.37	0.35
Case 2	0.10	0.15	0.50	0.25
Case 3	0.30	0.30	0.25	0.15

Table 4
Variations in injection gas composition.

Inj. comp.	C1	CO2	C4	C10
Case 1	0.97	0.01	0.01	0.01
Case 2	0.85	0.13	0.01	0.01
Case 3	0.80	0.18	0.01	0.01

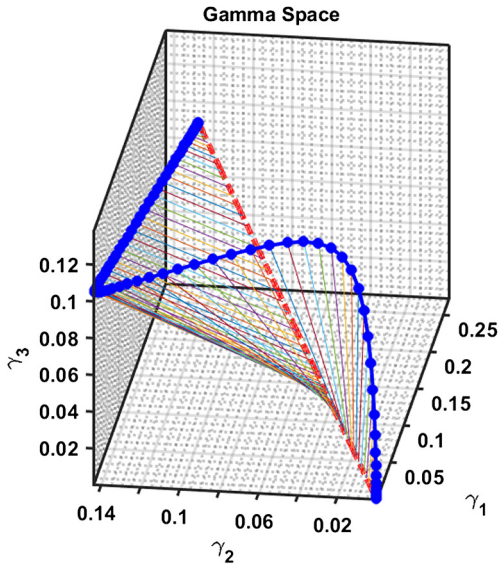


Fig. 9. Parameterized space (γ-path) for five-component system.

Nomenclature

Symbol	Description	Units
k	Absolute permeability	Darcy
μ_g	Viscosity of gas	Pa S
μ_o	Viscosity of oil	Pa S
ρ_g	Density of gas	Kg/m^3
ρ_o	Density of oil	Kg/m^3
ϕ	Porosity	–
K_i	Equilibrium ratio of component i	–
v	Mole fraction of vapor phase	Mol Fr
L	Mole fraction of liquid phase	Mol Fr
γ	Tie-line parameter	–
f_g	Fractional flow of gas phase	–
F_i	Fractional flow of component i	–
S_g	Saturation of gas	–
S_o	Saturation of oil	–
λ_j	Mobility of phase j	–
u_j	Darcy velocity of phase j	m/s
Λ	Shock velocity	m/s
x_i	Composition of component i in liquid phase	Molar Fraction
y_i	Composition of component i in vapor phase	Molar Fraction
z_i	Overall composition of component i	Moles
p	Pressure	N/m^2
σ	Parameterized variable	–
n_c	Number of components	–
n_p	Number of phases	–

Acknowledgement

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Table 5
Reservoir fluid properties.

Properties	Gas	Oil
Residual saturation (S_{jr})	0.0	0.0
End point relative perm. (K_{rej})	1.0	1.0
Saturation exponent (n_j)	2.0	2.0
Phase viscosity in cP (μ_j)	1.0	5.0

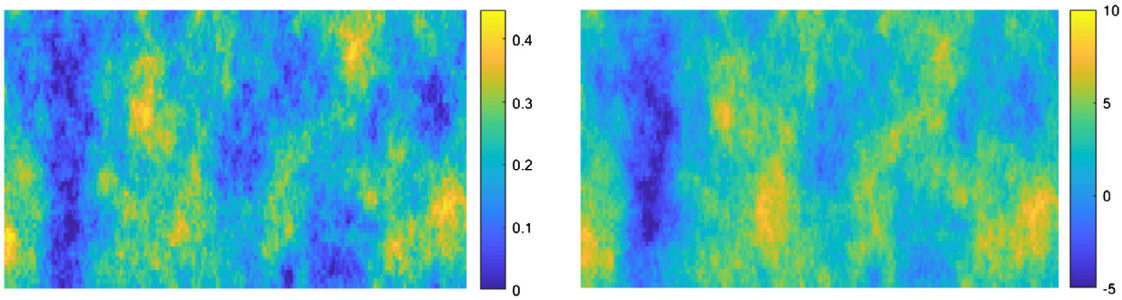


Fig. 10. Upper layer of SPE10 test case: (a) porosity and (b) log of permeability.

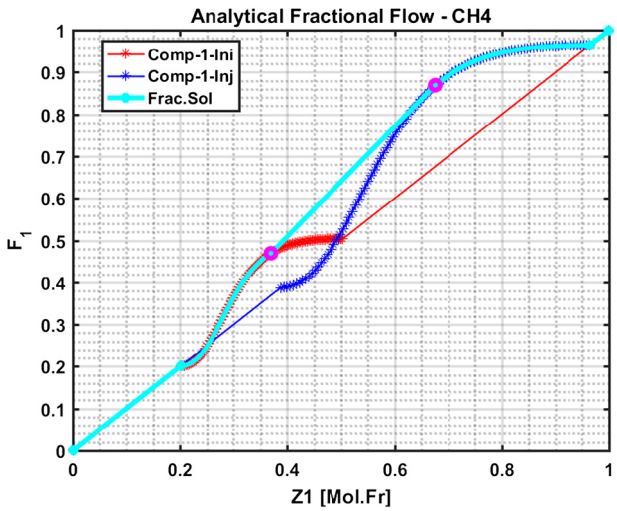


Fig. 11. Analytical fractional flow curve based on non-tie-line rarefaction.

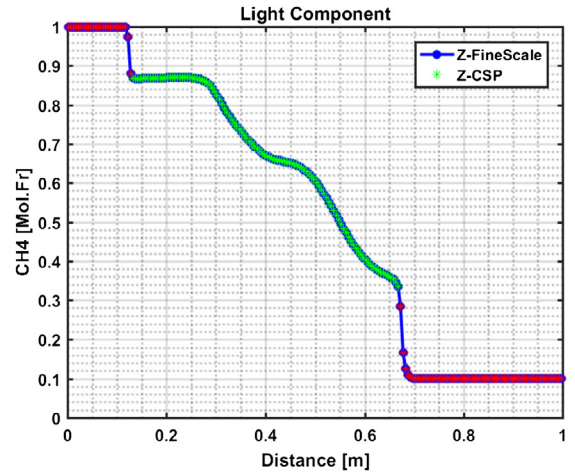
Appendix A

A.1. Simulation parameters

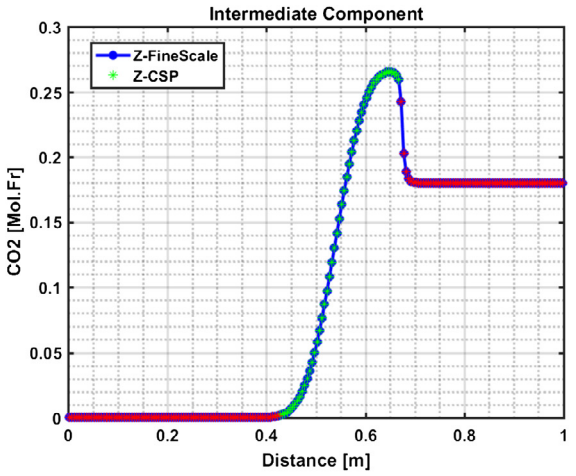
In this Appendix, we present simulation parameters for all performed simulations in addition to the parameters already described in the result section.

A.2. Non tie-line rarefaction

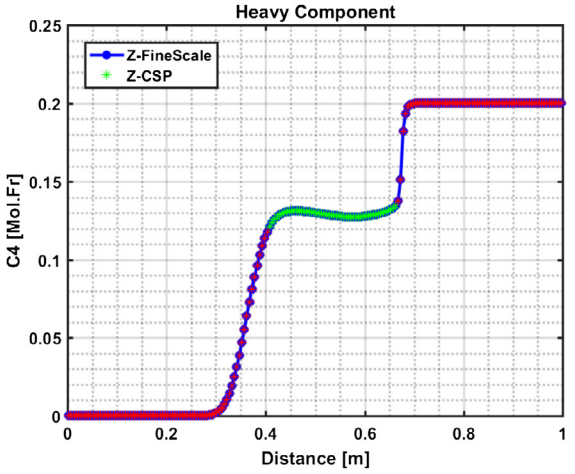
The construction of a fractional flow solution curve is similar to the construction of a compositional path, which in turn is generally represented by a series of shocks and rarefaction (both tie-line and non-tie-line). Based on this, the fractional flow solution curve (Frac.Sol curve in Fig. 11) is constructed in compliance with the conservation laws as shown in below. The cardinal difference between the traced solution curve, implemented in the conventional simulation, and the one shown here is related to the path of non-tie-line rarefaction (indicated by the straight line in between the tangent dots). Though the traced solution curve indicated above ensures conservation, on the other hand, locating these points on the curve makes the approach cumbersome. Hence the solution curve is constructed by tracing the injection and the initial flow curves with a switch at their point of intersection, without tracing the non-tie-line path (since it is sufficient enough to accurately



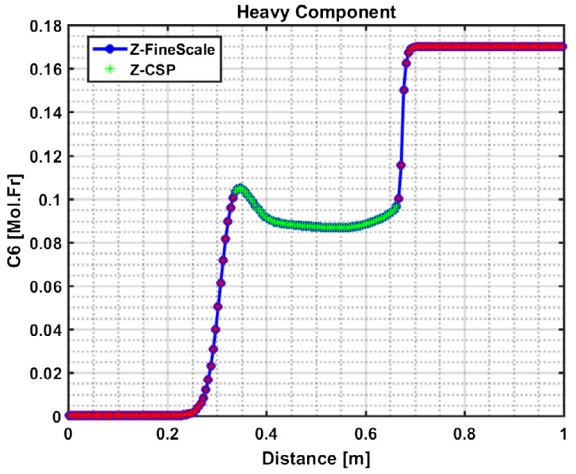
(a)



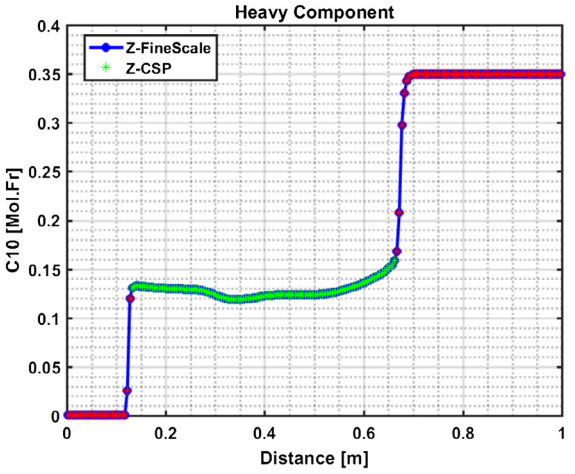
(b)



(c)



(d)



(e)

Fig. 12. Reconstructed two-phase region of 5C system, vaporizing gas drive (a) light component CH_4, (b) first intermediate component CO_2, (c) second intermediate component C_4, (d) third intermediate component C_6, (e) heavy component C_{10}.

construct or trace the fractional flow solution curve with respect to the shock regions). As a result, the solution profile within the two-phase region is sporadic.

A.3. Reconstruction of 5C system

The modified transport equation based on the CSP technique is solved over the 3D parameterized space (as shown in Fig. 9) and the corresponding results of reconstruction are shown in Fig. 12. Based on the plots, we can conclude that the proposed technique yields exact results as that of a conventional fine-scale simulation. Also, the results reinstate the fact that the developed multiscale approach results in coarsening of system representation, thereby enhancing the performance.

References

[1] K. Aziz, T. Settari, Petroleum Reservoir Simulation, Applied Science Publishers, 1979.
[2] M. Michelsen, The isothermal flash problem. Part I. Stability, Fluid Phase Equilib. 9 (1) (1982) 1–19.
[3] M. Michelsen, The isothermal flash problem. Part II. Phase-split calculation, Fluid Phase Equilib. 9 (1) (1982) 21–40.
[4] K. Coats, An equation of state compositional model, SPE J. 20 (05) (1980) 363–376.
[5] T. Hou, X.-H. Wu, A multiscale finite element method for elliptic problems in composite materials and porous media, J. Comput. Phys. 134 (1) (1997) 169–189, https://doi.org/10.1006/jcph.1997.5682.
[6] P. Jenny, S. Lee, H. Tchelepi, Multi-scale finite-volume method for elliptic problems in subsurface flow simulation, J. Comput. Phys. 187 (1) (2003) 47–67, https://doi.org/10.1016/S0021-9991(03)00075-5.
[7] Y. Efendiev, V. Ginting, T. Hou, R. Ewing, Accurate multiscale finite element methods for two-phase flow simulations, J. Comput. Phys. 220 (1) (2006) 155–174, https://doi.org/10.1016/j.jcp.2006.05.015.
[8] H. Hajibeygi, G. Bonfigli, M. Hesse, P. Jenny, Iterative multiscale finite-volume method, J. Comput. Phys. 227 (19) (2008) 8604–8621, https://doi.org/10.1016/j.jcp.2008.06.013.
[9] O. Møyner, K.-A. Lie, A multiscale restriction-smoothed basis method for high contrast porous media represented on unstructured grids, J. Comput. Phys. 304 (2016) 46–71.
[10] S. Shah, O. Møyner, M. Tene, K.-A. Lie, H. Hajibeygi, The multiscale restriction smoothed basis method for fractured porous media (f-msrsb), J. Comput. Phys. 318 (2016) 36–57.
[11] H. Zhou, S. Lee, H. Tchelepi, Multiscale finite-volume formulation for saturation equations, SPE J. 17 (01) (2012) 198–211.
[12] M. Cusini, B. Fryer, C. van Kruijsdijk, H. Hajibeygi, Algebraic dynamic multilevel method for compositional flow in heterogeneous porous media, J. Comput. Phys. 354 (2018) 593–612, https://doi.org/10.1016/j.jcp.2017.10.052.
[13] G.I. Barenblatt, V.M. Entov, V.M. Ryzhik, Theory of Fluids Flow Through Natural Rocks, Springer Science and Business Media Dordrecht, 1990, Series ISSN 0924-6118, Hardcover ISBN 978-0-7923-0167-7, Softcover ISBN 978-90-481-4042-8.
[14] D. Tang, A. Zick, A new limited compositional reservoir simulator, in: SPE Symposium on Reservoir Simulation, Society of Petroleum Engineers, 1993.
[15] F. Helfferich, Theory of multicomponent, multiphase displacement in porous media, SPE J. 21 (01) (1981) 51–62.
[16] W. Monroe, M. Silva, L. Larson, F.J. Orr, Composition paths in four-component systems: effect of dissolved methane on 1D CO2 flood performance, SPE Reserv. Eng. 5 (03) (1990) 423–432.
[17] R. Johns, B. Dindoruk, F.J. Orr, Analytical theory of combined condensing/vaporizing gas drives, SPE Adv. Technol. Ser. 1 (02) (1993) 7–16.
[18] F.M. Orr Jr., Theory of Gas Injection Processes, Tie-Line Publications, 2007, ISBN 87-989961-2-5.
[19] P. Bedrikovetsky, M. Chumak, Riemann problem for two-phase four-and morecomponent displacement (ideal mixtures), in: ECMOR III-3rd European Conference on the Mathematics of Oil Recovery, 1992.
[20] D. Voskov, V. Entov, Problem of oil displacement by gas mixtures, Fluid Dyn. 36 (2) (2001) 269–278.
[21] D. Voskov, H. Tchelepi, Compositional space parameterization: theory and application for immiscible displacements, SPE J. 14 (03) (2009) 431–440.
[22] A. Pires, P. Bedrikovetsky, A. Shapiro, A splitting technique for analytical modelling of two-phase multicomponent flow in porous media, J. Pet. Sci. Eng. 51 (1) (2006) 54–67.
[23] R. Zaydullin, D. Voskov, H. Tchelepi, Nonlinear formulation based on an equation-of-state free method for compositional flow simulation, SPE J. 18 (02) (2012) 264–273.
[24] H. Kazemi, C.R. Vestal, G. Shank, Efficient multicomponent numerical simulator, Soc. Pet. Eng. AIME J. 18 (5) (1978) 355–368.
[25] L. Nghiem, D. Fong, K. Aziz, Compositional modeling with an equation of state, SPE J. 21 (6) (1981) 687–698.
[26] K. Coats, Impes stability: selection of stable timesteps, SPE J. 8 (2) (2003) 181–187, https://doi.org/10.2118/84924-PA.
[27] G. Thomas, D. Thurnau, Reservoir simulation using an adaptive implicit method, SPE J. 23 (5) (1983) 759–768, https://doi.org/10.2118/10120-PA.
[28] T.F. Russell, Stability Analysis and Switching Criteria for Adaptive Implicit Methods Based on the CFL Condition, Society of Petroleum Engineers, January 1, 1989.
[29] R. Courant, K. Friedrichs, H. Lewy, Über die partiellen differenzengleichungen der mathematischen physik, Math. Ann. 100 (1) (1928) 32–74, https://doi.org/10.1007/BF01448839.
[30] H. Cao, Development of Techniques for General Purpose Simulators, PhD Thesis, Stanford University, 2002.
[31] R. de Loubens, A. Riaz, H.A. Tchelepi, Error analysis of an adaptive implicit scheme for hyperbolic conservation laws, SIAM J. Sci. Comput. 31 (4) (2009) 2890–2914, https://doi.org/10.1137/080724502.
[32] C. Whitson, M. Michelsen, The negative flash, Fluid Phase Equilib. 53 (1989) 51–71.
[33] A. Iranshahr, D. Voskov, H. Tchelepi, Generalized negative-flash method for multiphase multicomponent systems, Fluid Phase Equilib. 299 (2) (2010) 272–284.
[34] D. Voskov, An extended natural variable formulation for compositional simulation based on tie-line parameterization, Transp. Porous Media 92 (3) (2012) 541–557.
[35] M. Christie, M. Blunt, Tenth SPE comparative solution project: a comparison of upscaling techniques, SPE Reserv. Eval. Eng. 4 (4) (2001) 308–316.
[36] D. Voskov, Operator-based linearization approach for modeling of multiphase multi-component flow in porous media, J. Comput. Phys. 337 (2017) 275–288, https://doi.org/10.1016/j.jcp.2017.02.041.
[37] M. Khait, D. Voskov, Operator-based linearization for general purpose reservoir simulation, J. Pet. Sci. Eng. 157 (2017) 990–998.
[38] V. Entov, F. Turetskaya, D. Voskov, On approximation of phase equilibria of multicomponent hydrocarbon mixtures and prediction of oil displacement by gas injection, in: ECMOR VIII-8th European Conference on the Mathematics of Oil Recovery, 2002.