Multiscale reconstruction of compositional transport

Ganapathy, C.; Chen, Y.; Voskov, D.

DOI
10.3997/2214-4609.201802182

Publication date
2018

Document Version
Final published version

Published in
16th European Conference on the Mathematics of Oil Recovery, ECMOR 2018

P052

Multiscale Reconstruction Of Compositional Transport

C. Ganapathy (TU Delft), Y. Chen* (TU Delft), D. Voskov (TU Delft / Stanford University)

Summary

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, thereby making them computationally demanding. In an effort to enhance the solution strategy of the hyperbolic problem, we herewith propose a multiscale reconstruction of compositional transport problem. Until recently, multiscale techniques have been seldom implemented on transport equations. Here, 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 single transport equation is implemented with the objective of reconstructing the leading and trailing shock positions in space. The prediction of front propagation is the most critical aspect of the approach, as they involve a lot of uncertainty. Once their positions are identified, the full solution lying in the regions outside the shocks can be conservatively reconstructed based on the prolongation interpolation operator. Subsequently, 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 (based on Compositional Space Parameterization technique). We demonstrate applicability of the approach for the idealistic 1D test cases involving various gas drives with different number of components. Further, the first stage reconstruction was tested successfully on more realistic problems based on implementation in recently developed Operator-Based Linearization (OBL) platform.

Introduction

A compositional model is an essential and significant tool in understanding the subsurface processes. The modeling of this multiphase multicomponent displacement requires the numerical solution of the associated nonlinear system of governing equations. Also, an equations of state (EoS) model (Coats, 1980; Aziz and Wong, 1989; Chien et al., 1985) is generally employed to describe the phase behavioral changes happening in the system, which includes determining the number of phase state present and the composition split in each phases. In addition to the complexity of these computations, the number of equations that needs to be solved in each discretized cell and in each iterations are considerably large, thereby making compositional solvers computationally intensive and demanding.

One possibility to improve the performance of simulation is to apply multi-scale approach. It helps to reconstruct a fine-scale solution close to the cost of a coarse-scale solution with controlled error in accuracy. Various multi-scale methods have been developed for reservoir simulation. Amongst them, Multi-Scale Finite Volume (MSFV) methods have become a state of the art in modern reservoir simulation (Jenny et al., 2003; Hajibeygi et al., 2008), 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 equations), without improving the solution of hyperbolic part (transport equations with respect to saturation or composition). The work by Zhou et al. (2012) serves as a rare example where they reconstruct saturation of immiscible transport problem using different operators based on the heuristic-driven front tracking. Another possibility is to use an adaptive mesh refinement based on an algebraic multi-scale solution as shown in Cusini et al. (2018).

Profound efforts have been taken in the past to understand the behavior of hyperbolic problem (solution of compositional transport) based on pseudo-ternary representation (Barenblatt et al., 1990; Tang and Zick, 1993). This simplification is valid for several practical application as shown in Helfferich (1981). Further, important principles were also formulated regarding the compositional path - where it was shown that the solution path enters and exits the multiphase region as shocks. It was also proven that in two phases, these shocks coincides with the tie-line corresponding to an extension passing through injection and initial solutions (Helfferich, 1981). These ideas led to the development of a unified Method of Characteristics (MOC) framework for two-phase gas injection processes (Monroe et al., 1990; Johns et al., 1993) which was later extended to three-phase systems by LaForce et al. (2008a). In the limit of a dispersion free 1D displacement, it was proven that the entire compositional path is controlled by the key tie-lines of the system. It was also shown that the structure of tie-lines dictates the solution route in the compositional space (Orr, 2007). For multicomponent systems with more than two phases, is was also proven that the main shocks, connected initial and injection composition with multiphase region, are always belongs to an extension of the tie-simplex hyperplane defined by equilibrium (LaForce et al., 2008b; Voskov and Tchelepi, 2009b).

Based on these insights, a general approach for solving a compositional problem with the assumption of constant partitioning coefficients was proposed in (Bedrikovetsky and Chumak, 1992). This approach used the fact that the structure of 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 (Voskov and Entov, 2001), where the original compositional problem was projected onto a tie-line space, and later, the parameters pertaining to two-phase region of EoS based system are determined by polynomial approximations.

Subsequently, further developments have been made in determining the solution of compositional problem in the tie-line space. It was proven that the projection of solution to the tie-line space is invariant to the hydrodynamic parameters of the problem (Pires et al., 2006). The multi-linear interpolation techniques was utilized to represent the thermodynamic phase behavior of the multicomponent system which was referred as the Compositional Space Parameterization (CSP) (Voskov and Tchelepi, 2008). The CSP ideology eventually led to the development of Compositional Space Adaptive Tabulation (CSAT) method (Voskov and Tchelepi, 2009a), where the tie-lines are stored in a table and later looked up to obtain the

phase state of 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. These techniques not only accelerated the phase behavior computations, but also provided the basis for development of fully EOS-free compositional simulation approach (Zaydullin et al., 2012).

In this study, we propose a two-stage multi-scale strategy for constructing the solution of a compositional problem. We introduce two different sets of multi-scale operators based on the dynamics of hyperbolic problem. Initially, a fine scale restriction operator based on MOC theory (Orr, 2007) is applied to reduce the number of conservation equations to a single transport equation, thereby helping us to reconstruct boundaries of the two-phase region. Once these boundaries are identified, the full multicomponent solution in single-phase regions is reconstructed using an interpolation-based prolongation operator. The stage one reconstruction attributing to the identification of the phase boundaries were validated on a constant K-value based system, EoS based system and 2D heterogeneous reservoir model (SPE 10). It is worth observing that the EoS based system and 2D reservoir model (SPE 10) was implemented based on the Operator-Based Linearization (OBL) framework proposed in Voskov (2017). In OBL method, the terms of the discretized governing equations are factorized into space and state depended operators. The state-dependent operators are adaptively discretized in parameter space of the problem and multi-linear interpolation is applied for continuous representation (Khait and Voskov, 2017). Subsequently, in the second stage, 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 (CSP) technique (Voskov and Tchelepi, 2008).

The paper is organized as follows: a brief overview about the standard compositional simulation approach is described initially. Then the structure and procedure attributing to the multi-scale reconstruction strategy of compositional problem is described comprehensively. Further, their application to multicomponent gas injection problems are validated. Finally, the conclusion and future scope are described in the last section.

Conventional Modeling Approach

A structured approach constituting of two broad segments - namely the thermodynamic part and the hydrodynamic part is employed in solving a compositional problem. The thermodynamic computations describes the phase behavior of the system on the basis of phase stability test (Michelsen, 1982a) - to identify the existence of number of phase in a particular grid cell and flash calculation (Michelsen, 1982b) - to determine the split fraction of components amongst the phases present. It is worth noticing that, 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 both approaches to perform flash calculations. In a K-value based or on SSI iteration of flash calculation (Michelsen, 1982b), the general phase split procedure is reduced to the solution of the following equation:

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

The nonlinear equ. (1) is also referred as the Rachford-Rice equation (Whitson and Michelsen, 1989), which can be solved by a combination of bisection and Newton's method to determine the vapor phase fraction (v). Further, the flash calculation is not limited to two phase mixtures alone, as they can also be performed on single phase compositions (Whitson and Michelsen, 1989). Such a phase computation is generally referred to as the negative-flash calculation (Whitson and Michelsen, 1989; Iranshahr et al., 2010), where the equ. (1) 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 can be represented as a linear combination of phase composition, as they always lie 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.

Further, the hydrodynamic computations corresponds to the solution of flow and transport equations, thereby determining the pressure (p) and compositional changes (z). For an isothermal compositional

system consisting of n_c components and 2 phases (vapor and liquid), the transport equation is given by,

$$\frac{\partial}{\partial t}\phi\left[(x_i\rho_o S_o)+(y_i\rho_g S_g)\right]+\nabla\cdot\left[(x_i\overline{u_o}\rho_o)+(y_i\overline{u_g}\rho_g)\right]+\left[(x_i\rho_o q_o)+(y_i\rho_g q_g\right]=0,\ i=1,\ldots,n_c. \tag{2}$$

The fluid phase velocity (momentum conservation) is given by Darcys law as shown in equ. (3):

$$\overline{u_j}=-\overline{\overline{K}}\frac{k_{rj}}{\mu_j}\nabla p,\quad j=1,2. \tag{3}$$

For a 1D incompressible and isothermal reservoir (neglecting capillarity, diffusion and chemical reactions), the governing mass conservation equation can be simplified as shown in equ. (4).

$$\frac{\partial z_i}{\partial t}+\frac{u_t}{\phi}\frac{\partial F_i}{\partial x}=0,\quad i=1,\ldots,n_c. \tag{4}$$

Here z_i is defined as

$$z_i=\frac{x_i\rho_o S_o+y_i\rho_g S_g}{\rho_o S_o+\rho_g S_g}, \tag{5}$$

and can be found from the vapor fraction

$$v=\frac{\rho_g S_g}{\rho_o S_o+\rho_g S_g}, \tag{6}$$

which yield

$$z=x_i(1-v)+y_i v. \tag{7}$$

Additional constraints between the components and the phases exist under the statement of instantaneous thermodynamic equilibrium, thereby enabling us to close the system of equations, and the same is defined as equality in fugacity of vapor and liquid phases.

$$f_{i,g}(P,T,y_i)=f_{i,o}(p,T,x_i). \tag{8}$$

The fugacity is a function of pressure (p), temperature (T) and the phase compositions ($x_{i,j}$), and they are generally determined based on the equations of state (EoS). Subsequently, the auxiliary relations used in closing the system of equations are described as follows,

$$\sum_{i=1}^{n_c}x_i-1=0\quad\&\quad\sum_{i=1}^{n_c}y_i-1=0, \tag{9}$$

$$S_o+S_g=1. \tag{10}$$

Multi-scale modeling approach

With the aim of attaining better understanding of the proposed multi-scale technique, this section discusses the technicalities involved in the construction of compositional path (solution profile). Fig. 1 shows the solution for a 3 component system. Now, the compositional path is defined as the trajectory describing the compositional changes between the initial oil composition and the injected gas composition. The salient principles that governs its construction 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 consistent with the previously described principles (conservation equations).

On the other hand, the fractional flow theory provides insight on the mobility of the phases present, Fig. 1(b) is showing a plot of fractional flow curve. The velocity of each composition along the curve follows a simple rule - the characteristic velocity should monotonically increase from injection to initial composition. To satisfy this condition, the consistent solution should contain two shocks connecting initial and injection compositions and it is generally independent from the number of components present

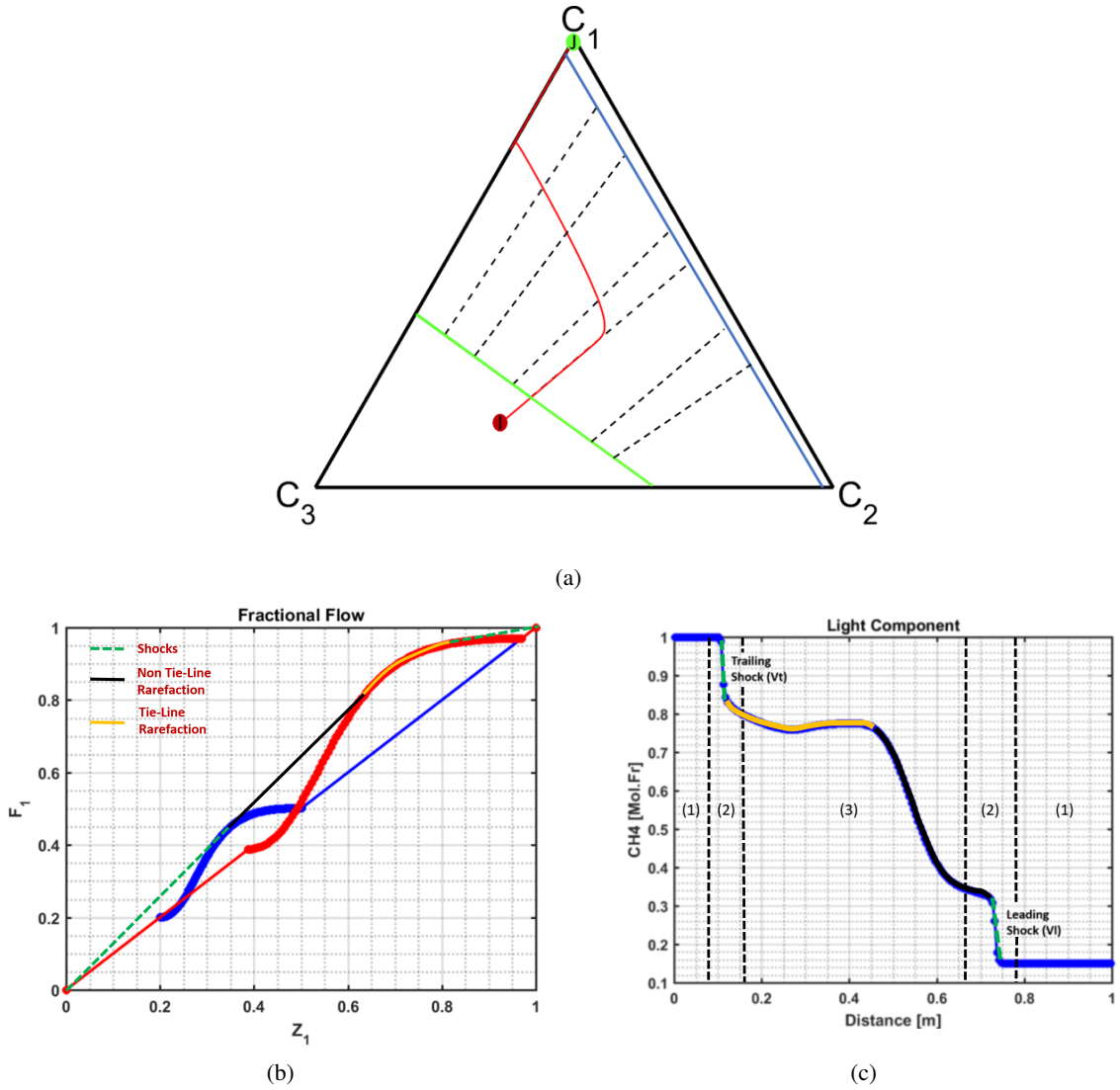


Figure 1 *General structure of compositional solution: (a) ternary phase diagram, (b) fractional flow curve, (c) solution profile (light component).*

in the system (Helfferich, 1981; Johns et al., 1993). These two shocks are generally referred as the leading and trailing shocks. 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 (Tang and Zick, 1993). Between these two shocks is the fan of characteristics associated with the continuous variation of composition, which is also known as the spreading or rarefaction waves. Also, a better understanding on the shock solution is given based on the Rankine-Hugoniot condition (Helfferich, 1981), which is given by the equ. (11):

$$\Lambda = \frac{dF_i}{dZ_i} = \frac{F_{i,2} - F_{i,1}}{Z_{i,2} - Z_{i,1}} \quad i = 1, \ldots, n_c \tag{11}$$

where, $F_{i,1}$ and $z_{i,1}$ represents the fractional flow and composition of component i on the downstream side of the shock and $F_{i,2}$ and $z_{i,2}$ represent the fractional flow and composition of component i on the upstream of the shock. The Rankine-Hugoniot condition is an integral version of the conservation equation shown in equ. (4) and it illustrates the fact that the volume is conserved across the shock.

The basis of the proposed multi-scale based reconstruction technique is attributed to the solution structure of the compositional problem Fig. 1(c), where the solution can be classified into three distinctive

regions based on the characteristic changes (Zhou et al., 2012). Here, 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 definitive jump in the saturation values. The characteristics of this region is defined based on the Rankine-Hugoniot condition (equ. (11)). Finally, region 3 refers to fan characteristics (rarefaction), where the saturation changes are more continuous. In summary, region 1 and region 3 are referred as "single phase region" and "two phase region" respectively, while region 2 is a "transition zone".

Based on the described perspective, it can be understood that the shock separates two contrasting zone of saturations, with these zones lying on either side of it (i.e) region 1 and region 3. This fact lays down the basis of the proposed multi-scale technique, where specially constructed restriction and prolongation operators are implemented on different regions of compositional changes to reconstruct the solution of the hyperbolic problem (full system). In the first stage, we reconstruct the position of shock in space as they hold the key. The same is being carried out using a fine scale restriction operator. Once the position of shocks are identified, the interpolation-based prolongation operator is applied to reconstruct the solution in single phase regions similar to the approach suggested in (Zhou et al., 2012). In the second stage, the solution for n_c components lying in between the leading and trailing shocks is reconstructed with the aid of the restriction and prolongation operators defined based on CSP technique (Voskov and Tchelepi, 2009a).

Both vaporizing and condensing gas drives have been implemented based on the suggested multi-scale framework, and the details of the injection gas and initial oil compositions are given in Appendix C. On the other hand, the hydrodynamic parameters used during simulation are as follows: Porosity (ϕ)=0.3, Oil viscosity (μ_o)=5cP, Gas viscosity(μ_g)=1cP, Saturation exponent of oil(n_o) and gas(n_g) =2, End point relative permeability of oil(K_{reo}) and gas(K_{reg})=1 respectively.

Multi-scale reconstruction of single-phase regions

The tracking of front propagation for a compositional transport problem is carried out based on analytically constructed pseudo fractional flow curves, which in turn play the role of restriction operator. At first, the liquid (x_i) and the vapor (y_i) fraction values of the compositions lying on the extension of injection and initial tie-line (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 2-phase region based on

$$F_i = x_i(1-f_g) + y_i f_g, \qquad i = 1,\ldots,(n_c-1). \tag{12}$$

Within the 2-phase region, the fractional flow plot is an S-shaped curve. In the single phase region,

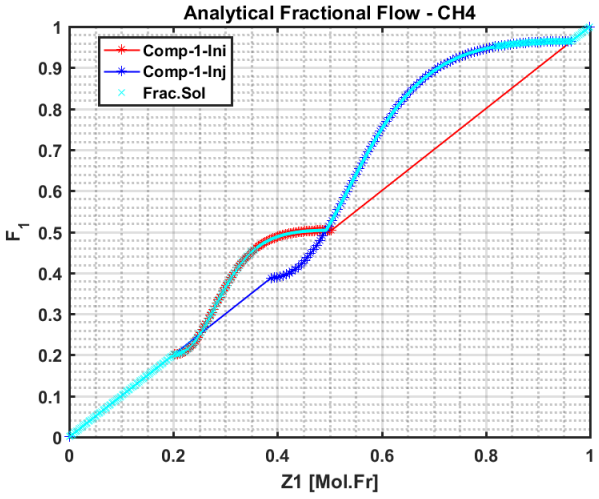


Figure 2 *Analytical fractional flow curve, representing light component (C_1).*

the fractional flow value of a particular component varies linearly with the molar fraction of the corresponding component itself. 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 on the injection and initial tie-lines of the system, they are eventually combined together and an equivalent restriction transport operator 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 constructed curve shown in Fig. 2 represents the pseudo-fractional-flow curve for the reconstruction of leading and trailing shocks. These values are tabulated and defined as restriction operator during the course of 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:

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

Validation for K-value-based system

Fig. 3 exhibits the reconstructed shock solution for a four-component system (vaporizing gas drive). The results of the reconstructed solution is assessed by comparing it with a reference compositional solution. It can be noticed that the shock positions are accurately reconstructed to fine scale accuracy with the use

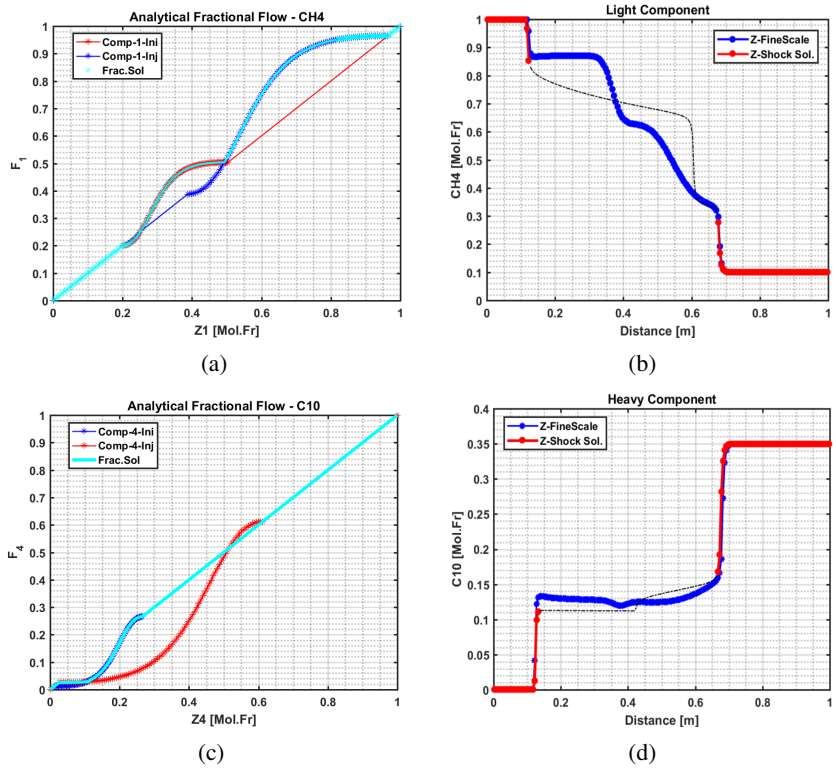


Figure 3 *Analytical fractional flow curves along with reconstructed shock positions for (a),(b) light component-(C_1), (c),(d) heavy component (C_{10}).*

of the restriction operator. On the other hand, the solution between the shocks (in the two-phase region) differs with the fine scale solution. Though there is a valid reason behind this mismatch (see discussion in Appendix A), this difference can be neglected since our objective is limited to the accuracy of shock reconstruction. In this stage, our multi-scale approach reduces the complexity (number of equations solved per control volume) from $(n_c - 1)$ transport equations to one.

Once the phase boundaries are identified, the solution lying in the singe phase region is reconstructed by applying the interpolation-prolongation operator as defined mathematically in

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

where, $\boldsymbol{\kappa}$ is the interpolation-prolongation operator, z_R is the reconstructed shock solution and $\mathbf{I}$ is the piecewise-linear interpolation function. The prolongation operator is based on interpolation of an entire solution between injection and initial composition using the concentration of pseudo-component from the solution of restricted problem. 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.11. Conceptually, this approach is similar to the prolongation operation for reconstruction of fine scale spatial solution proposed in (Zhou et al., 2012).

Multi-scale reconstruction using OBL framework

In this section, we briefly describe the Operator-Based Linearization (OBL) approach (Voskov, 2017) which is used for the extension of the first-stage multi-scale reconstruction to EoS-based and 2D simulation later. The more general set of governing compositional equations is solved in combination with the restriction operator implemented in OBL. Applying two-point finite-volume in space and backward Euler in time discretization to equ.(2), the general mass conservation equation is written as:

$$V\left(\left(\phi\sum_{j=1}^{2}x_{i,j}\rho_j S_j\right)^{n+1} - \left(\phi\sum_{j=1}^{2}x_{i,j}\rho_j S_j\right)^{n}\right) - \Delta t\sum_{l\in\mathbf{L}}\left(\sum_{j=1}^{2}x_{i,j}^{l}\rho_j^{l}T_j^{l}\Delta\Psi^{l}\right) + V\Delta t\sum_{j=1}^{2}x_{i,j}\rho_j q_j = 0, \tag{17}$$

where V is total control volume. Here, $\mathbf{L}$ represents the interface which connects the control volume with another grid blocks. To simplify the model, $\Delta\Psi^{l}$ means only pressure gradient between two connected grid blocks and T_j^{l} is the transmissibility of phase j. To apply OBL, the discretized mass conservation equation (equ.17) is written in the following residual form:

$$R_i(\xi,\omega,\mathbf{u}) = a(\xi)\left(\alpha_i(\omega) - \alpha_i(\omega_n)\right) - \sum_{v}\beta_i^{v}(\omega)b^{v}(\xi,\omega) + \theta_i(\xi,\omega,\mathbf{u}) = 0. \tag{18}$$

The operators in equ.(18) are defined as follows:

$$\alpha_i(\omega) = (1 + c_r(p - p_{ref}))\sum_{j=1}^{2}x_{i,j}\rho_j S_j, \tag{19}$$

$$a(\xi) = V(\xi)\phi_0(\xi), \tag{20}$$

$$\beta_i(\omega) = \sum_{j}^{2}x_{i,j}\frac{k_{rj}}{\mu_j}\rho_j, \tag{21}$$

$$b(\xi,\omega) = \Delta t T_{ab}(\xi)(p^b - p^a), \tag{22}$$

$$\theta_i(\xi,\omega,\mathbf{u}) = \Delta t\sum_{j=1}^{2}x_{i,j}\rho_j q_j(\xi,\omega,\mathbf{u}). \tag{23}$$

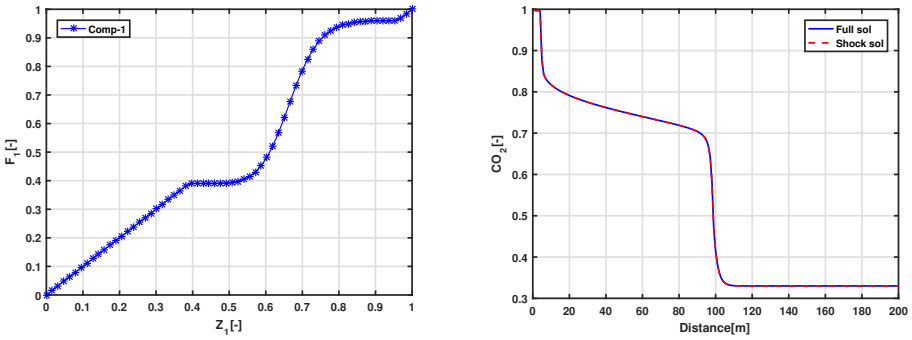
From equ.(19) to equ.(23), c_r is rock compressibility and T^{ab} is transmissibility of the reservoir. The vector $\mathbf{u}$ contains well control variables, ω is state variables and ξ are spatial coordinates. In addition,

α_i is the accumulation operator, β_i is the flux operator and θ_i is the source/sink operator. The OBL approach is based on a multi-linear interpolation of the nonlinear operators in the parameter space of the simulation problem, see Voskov et al. (2017) and Khait and Voskov (2017, 2018) for details. For an isothermal reservoir simulation, the parameter space is defined by pressure p ranging between injection and production conditions, and overall compositional z_i range from 0 to 1.

Validation for EOS-based system

In continuation to the previously described constant K-value implementation (Ganapathy, 2017), here we introduced the EoS-based methodology to determine the thermodynamic parameters. The validation of this reconstruction is carried out for a binary compositional system first and later for a quaternary system. In a binary system, the injection and initial tie-lines are equal for a fixed pressure due to the Gibbs phase rule. As a result, it implies that the first-stage reconstruction on a binary system yields the full solution of the problem.

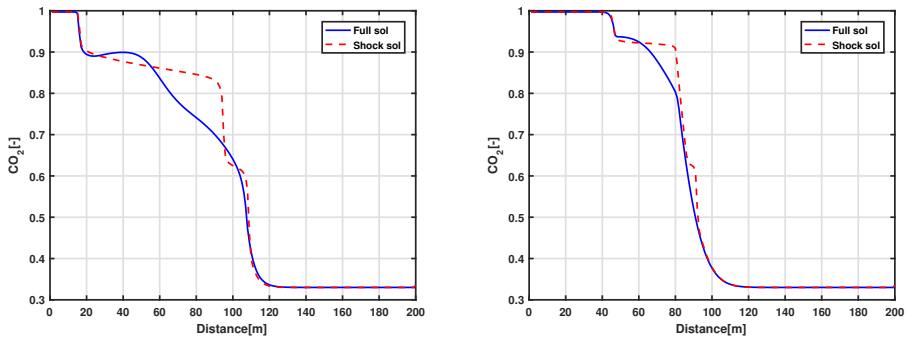
Initially, a single full scale fractional flow curve of CO_2 is determined. Taking the fractional flow dependency on CO_2 composition, a fine scale 1D two-component injection transport problem is solved. In this example, the temperature is 373K and the simulation time is defined as 1000 days. Fig 4(a) shows



(a) (b)

Figure 4 *First stage reconstruction of binary system: (a) fractional flow curve for CO_2 (b) full and reconstructed solution for CO_2.*

the fractional flow curve of CO_2 for a fixed pressure (100 bars) based on the EoS computations, and Fig 4(b) gives the solution for the full system along with the reconstructed shock solution. According to the theory, the displacement path of the binary system is along a single tie-line, thereby resulting in a single fractional flow curve. As a result, only the shock solution reconstruction framework is plausible to construct the full transport solution of a binary system.



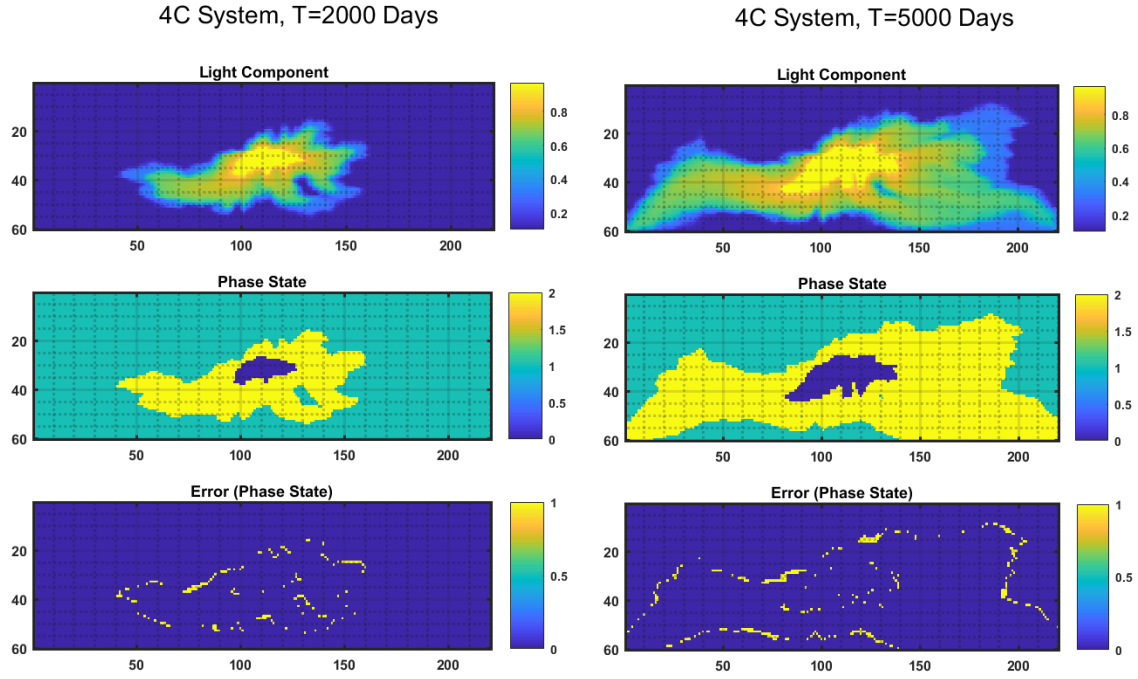
(a) 85bar (b) 120bar

Figure 5 *Shock reconstruction for a four-component system based on multiscale approach for different BHPs at producer (EoS based).*

Similar framework of reconstruction (based on EoS approach) was also applied for a quaternary system and the corresponding results of shock reconstruction are shown in Fig. 5, describing the compositional changes for growing bottom hole pressure (BHP) at producer. The injection gas and the initial oil composition used in the simulation are described in Appendix C.

Validation for 2D solution

In addition to the 1D validation, the proposed first stage reconstruction was also tested for highly heterogeneous reservoir characterization. For this test, the top layer of SPE 10 model with highly-heterogeneous porosity and permeability maps were used (Christie and Blunt, 2001). The model is built on a regular Cartesian grid (60 x 220 cells), with one gas injection well in the center and four production wells at corners. We applied a first-stage of the proposed multi-scale approach based on OBL technique.



(a) Solution after T=2000 days

(b) Solution after T=5000 days

Figure 6 *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.*

The pseudo-binary system was solved which yield a solution for pressure and indicator composition. The solution for the full system (n_c components) is reconstructed by linearly interpolating full set of compositions between the initial and the injection mixtures using the indicator composition. In other words, irrespective of the size of the system, a pseudo binary model is sufficient enough to determine the phase boundaries of a full n_c-component system.

Fig. 6 shows the reconstructed shock solution of SPE 10 model at different two steps, for vaporizing gas drive system described in Appendix C (with constant K-value). 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 mismatch in phase boundaries between the full conventional approach and the proposed multi-scale reconstruction demonstrates the profoundness of the methodology.

Multi-scale reconstruction of two-phase region

The solution in the two phase region is determined based on Compositional Space Parameterization technique (Voskov and Tchelepi, 2009a). 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 problem is largely controlled by the properties of a few key tie-lines that defines the structure of compositional solution, and hence it is advantageous to parameterize the problem based on these tie-lines. It has also been proven that the projection of compositional solution into the tie-line space is invariant to the changes in hydrodynamic properties (e.g. relative permeabilities), see Pires et al. (2006) for details.

Grounding on the methodology of parameterization, a novel simulation framework has been proposed for the solution of hydrodynamic problem, thereby reconstructing the solution in 2-phase region (Voskov and Entov, 2001). This reconstruction is based on the invariance of compositional solution in tie-line space. Notice that this technique requires either the solution of auxiliary thermodynamic problem (Entov et al., 2002), or the solution of full problem and its projection onto the tie-line space (Voskov and Tchelepi, 2009a).

Initially, the existing tie-lines of the solution are parameterized based on γ variables. It is worth noticing that the governing variables (γ) can be defined arbitrarily in the compositional space except for the fact that they should uniquely identify tie-lines. For instance, they can be defined as a tie-line trace on the face of compositional diagram (Voskov and Entov, 2001), or at a plane representing the tie-line centers (Voskov and Tchelepi, 2009a). The resulting Γ-path present discontinuities (shocks and rarefactions) associated with the key tie-lines of the solution, see example in Fig. 7. Here, γ_1 and γ_2 refer to the phase fractions of intermediate components in a four component system. Once the Γ-path is constructed, a

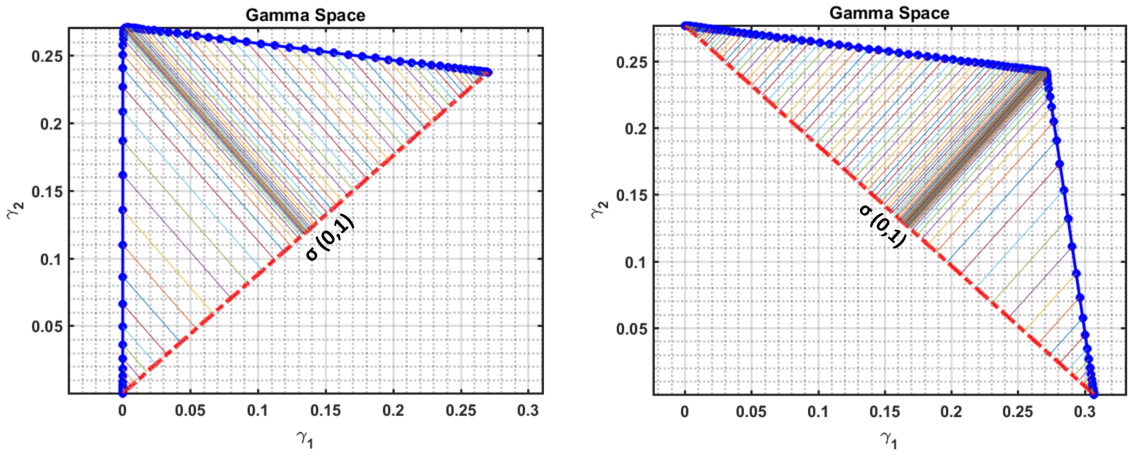


Figure 7 *Parametrization of solution in tie-line space (Γ-path): (a) vaporizing gas drive, (b) condensing gas drive.*

new variable σ is introduced. The objective of this σ variable is to parameterize the calculated Γ-path. In this study, we parameterize the entire solution in γ-space by orthogonally projecting values of γ onto the σ-line where σ is changing between 0 and 1 when γ is changing between injection and production tie-lines (Fig. 7). In this representation, all phase fractions become nonlinear with $x_i(\sigma)$ and $y_i(\sigma)$. Following this procedure, the compositional variation of the entire problem is parameterized in tie-line space. Notice that this solution is invariant to changes in hydrodynamic properties of the problem and depends only on thermodynamic properties and injection/initial conditions (Voskov and Entov, 2001; Pires et al., 2006). Now the solution for the 2-phase region (area within the leading and trailing shocks) is determined by solving the reduced transport problem in the parameterized space. First, we represent overall composition at new timestep through the nonlinear relation involving phase fractions:

$$z_i^{n+1} = y_i(\sigma^{n+1}) \cdot v^{n+1} + x_i(\sigma^{n+1}) \cdot (1 - v^{n+1}). \tag{24}$$

Now we can substitute this relation into two conservation equations (4) in discretized form. The resulting restricted conservation equations takes the following residual form:

$$R_i = y_i(\sigma^{n+1}) \cdot v^{n+1} + x_i(\sigma^{n+1}) \cdot (1 - v^{n+1}) - z^n - \frac{dt}{\phi \cdot dx} \{(F_i \cdot U_{i+1}) - (F_{i-1} \cdot U_i)\}^n \quad i = 1,2. \tag{25}$$

For simplicity, we are using here an explicit time approximation for the flux term and the same does not limit a general-purpose application of the proposed approach. The equ.(25) is nonlinear in nature even for an explicit flux approximation which is induced by the nonlinear dependency of tie-line parameters (x_i and y_i) on σ. As a result, the Newton's method has been applied to obtain the solution. It is also to be noted that the n_c variables of the original compositional problem is replaced by just two variables (σ and v) in the second stage reconstruction. In other words, the equ.(25) is solved with parameterized variable σ and vapor fraction v as its primary unknowns instead of directly solving for the overall compositions (z_i), thereby resulting in the restriction of full system. The final system of equations (in algebraic form) is given by,

$$\begin{bmatrix} \frac{\partial R_1}{\partial \sigma} & \frac{\partial R_1}{\partial v} \\ \frac{\partial R_2}{\partial \sigma} & \frac{\partial R_2}{\partial v} \end{bmatrix} \begin{bmatrix} \delta\sigma \\ \delta v \end{bmatrix} = \begin{bmatrix} -R_1 \\ -R_2 \end{bmatrix}. \tag{26}$$

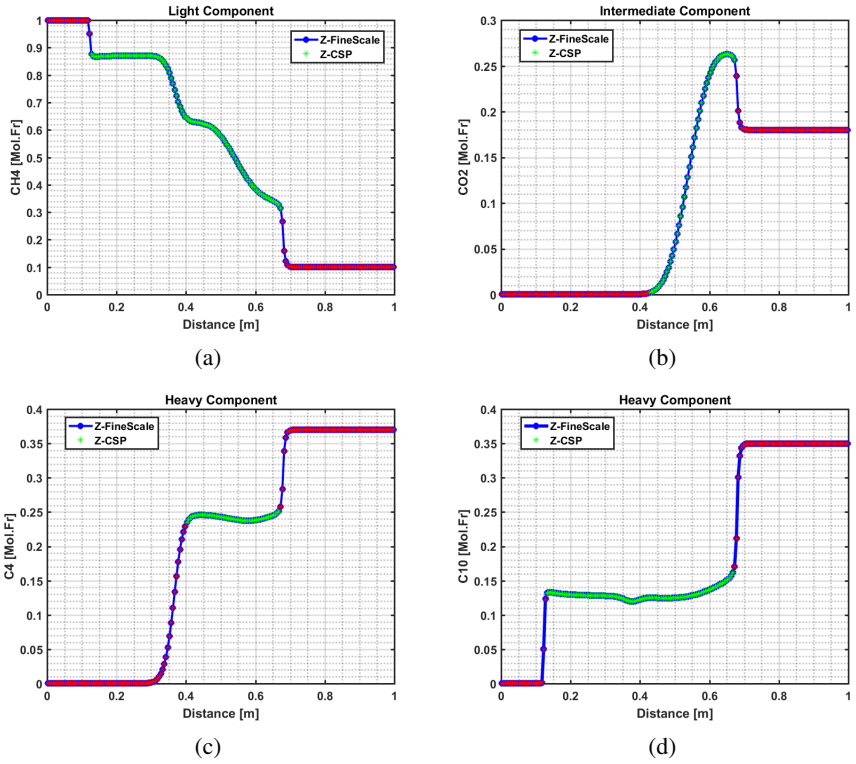


Figure 8 *Full reconstruction of four-component problem for vaporizing gas drive (a) light component C_1 (b) intermediate component CO_2 (c) heavier component C_4 and (d) heavy component C_{10}*

In the first stage of multi-scale reconstruction, the shock positions are located in space based on solution with restriction operator and compositions in single-phase region are reconstructed using prolongation operator based on interpolation. Now, the full solution in two-phase region is reconstructed by solving only two restricted conservation equations (25) in the parameterized space. Once the solution is obtained, the prolongation operator is applied again based on the projection of σ-solution (points on red curve) to Γ-path (points on blue curve), see figure 7 for details):

$$\boldsymbol{\psi}(\gamma,\sigma)\left[\mathbb{R}^2 \Longrightarrow \mathbb{R}^{n_c-1}\right] : \mathbf{z} = \mathbf{y}(\sigma)\cdot v + \mathbf{x}(\sigma)\cdot(1-v) \tag{27}$$

Notice that γ-parameters uniquely identify tie-lines in the compositional space, which defines the corresponding values of $\mathbf{x}$ and $\mathbf{y}$. Once tie-line is reconstructed based on σ, the corresponding overall compositions $\mathbf{z}$ are recovered using solution in v and equ. (27).

Fig. 8 and Fig. 9 describes the solution of a vaporizing and condensing gas drive. It is clear that the reconstructed two phase region (Z-CSP curve) accurately matches with the reference fine scale solution.

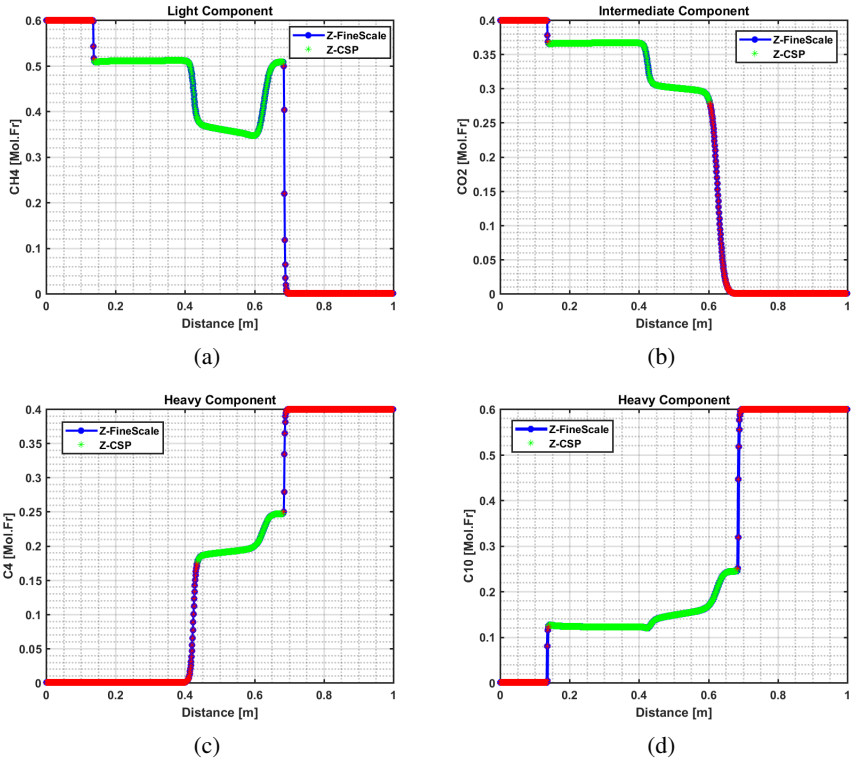


Figure 9 *Full reconstruction of four-component problem for condensing gas drive (a) Light Component CH_4 (b) Intermediate Component CO_2 (c) Heavy Component C_4 (d) Heavy Component C_{10}*

It is worth observing that the reconstructed solution of the entire $(n_c - 1)$ independent compositions are obtained by solving the restricted representation of the system (σ and v) in two-phase region only. 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 solution of black-oil problem. Also, the decoupling between the thermodynamic and hydrodynamic problems provides a simple platform to carry out multi-dimensional analysis and sensitivity studies, since the Γ-path is independent of flow properties and only depends on thermodynamic parameters of the system.

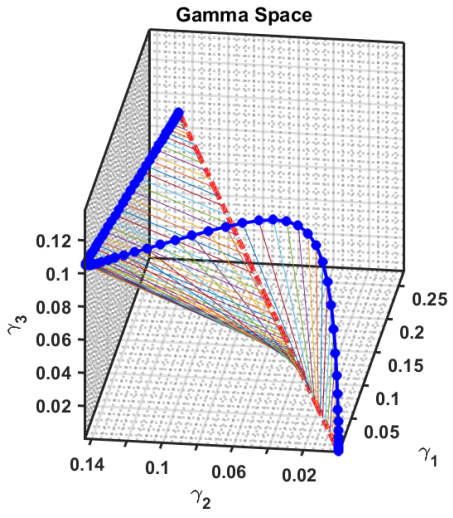


Figure 10 *Parameterized space (Γ-path) of 5C system.*

The parameterization technique stays legitimate, and is independent of the number of components. Moreover it is enough to solve the same restricted system of equations with v and σ as primary unknowns for any system with arbitrary number of components. The only difference is the dimension of the the γ-space, where the 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 (Voskov and Entov, 2001). For example, the Fig. 10 below shows the gamma path for a five-component system and the corresponding results of reconstruction are shown in Appendix B.

Conclusions

Through this research work, a novel multi-scale in physics approach has been proposed to enhance the efficiency of a compositional problem. The methodology is based on the local compositional profile of the system, and eventually a two-stage reconstruction of the compositional transport problem is carried out. In this study we present the application of the proposed technique for a compositional problem (multicomponent gas injection).

At first, we present the method for identifying the front (shock) positions in space using the restriction operator based on fractional flow theory. This approach was tested for several gas injection problems of practical interest, including K-values and full EoS-based multicomponent systems, and it accurately predicts boundaries of two-phase region. An interpolation-based prolongation operator was subsequently applied for the reconstruction of solution in the single-phase regions, thereby precisely matching the conservative solution of the full problem in this region.

The second stage of the proposed multi-scale 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 technique (CSP). The restriction operator reduces the full system of conservation equations to two equations per each control volume. 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 fine scale solution of full problem.

While the proposed multi-scale approach is found to be rewarding, there are several possibilities for its future extensions. An obvious and straightforward advancement would be to implement this technique in a fully implicit compositional framework involving complex nonlinear physics. Further, a similar approach can also be extended to thermal and chemical problems involving arbitrary number of phases.

Acknowledgements

We acknowledge the assistance and support extended by Mark Khait during the coarse of this work.

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_i	Fractional flow of component i	–
f_g	Fractional flow of gas phase	–
f_o	Fractional flow of oil phase	–
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	$Mol.Fr$
y_i	Composition of component i in vapor phase	$Mol.Fr$
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	–
V	Total control volume	m^3
$\mathbf{L}$	Interface connecting blocks	–
$\Delta\Psi^l$	Pressure difference	bar
α_i	Accumulation operator (component i)	–
β_i	Flux operator (component i)	–
θ_i	Source/sink operator (component i)	–
c_r	Rock compressibility	$1/bar$
T^{ab}	Transmissibility of block a and b	m^2
ω	State variables	–
ξ	Spatial coordinates	–

References

Aziz, K. and Wong, T. [1989] Considerations in the development of multipurpose reservoir simulation models. In: *proceedings of the 1st and 2nd International Forum on Reservoir Simulation, Alpbach, Austria*.

Barenblatt, G., Entov, V. and Ryzhik, V. [1990] Fluids flow through natural rocks. *Dordrecht, Kluwer*.

Bedrikovetsky, P. and Chumak, M. [1992] Riemann problem for two-phase four-and morecomponent displacement (Ideal Mixtures). In: *ECMOR III-3rd European Conference on the Mathematics of Oil Recovery*.

Chien, M., Lee, S. and W.H. Chen, W. [1985] A new fully implicit compositional simulator. In: *SPE Reservoir Simulation Symposium*. Society of Petroleum Engineers.

Christie, M. and Blunt, M. [2001] Tenth SPE comparative solution project: A comparison of upscaling techniques. *SPE Reservoir Evaluation and Engineering*, **4**(4), 308–316.

Coats, K. [1980] An equation of state compositional model. *SPE Journal*, **20**(05), 363–376.

Cusini, M., Fryer, B., van Kruijsdijk, C. and Hajibeygi, H. [2018] Algebraic dynamic multilevel method for compositional flow in heterogeneous porous media. *Journal of Computational Physics*, **354**, 593–612.

Entov, V., Turetskaya, F. and Voskov, D. [2002] 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*.

Ganapathy, C. [2017] *Multiscale Reconstruction of Compositional Transport*. Master's thesis, Delft University of Technology.

Hajibeygi, H., Bonfigli, G., Hesse, M. and Jenny, P. [2008] Iterative multiscale finite-volume method. *Journal of Computational Physics*, **227**(19), 8604–8621.

Helfferich, F. [1981] Theory of multicomponent, multiphase displacement in porous media. *SPE Journal*, **21**(01), 51–62.

Iranshahr, A., Voskov, D. and Tchelepi, H. [2010] Generalized negative-flash method for multiphase multicomponent systems. *Fluid Phase Equilibria*, **299**(2), 272–284.

Jenny, P., Lee, S. and Tchelepi, H. [2003] Multi-scale finite-volume method for elliptic problems in subsurface flow simulation. *Journal of Computational Physics*, **187**(1), 47–67.

Johns, R., Dindoruk, B. and Orr, F.J. [1993] Analytical theory of combined condensing/vaporizing gas drives. *SPE Advanced Technology Series*, **1**(02), 7–16.

Khait, M. and Voskov, D. [2017] Operator-based linearization for general purpose reservoir simulation. *Journal of Petroleum Science and Engineering*, **157**, 990–998.

Khait, M. and Voskov, D. [2018] Adaptive Parameterization for solving of Thermal/Compositional Nonlinear flow and transport with Buoyancy. *SPEJ*, **182685**.

LaForce, T., Jessen, K. and Orr, F. [2008a] Four-component gas/water/oil displacements in one dimension: Part I. Structure of the conservation law. *Transport in Porous Media*, **71**(2), 199–216.

LaForce, T., Jessen, K. and Orr Jr., F. [2008b] Four-component gas/water/oil displacements in one dimension: Part II, example solutions. *Transport in Porous Media*, **72**(1), 83–96.

Michelsen, M. [1982a] The isothermal flash problem. Part I. Stability. *Fluid phase equilibria*, **9**(1), 1–19.

Michelsen, M. [1982b] The isothermal flash problem. Part II. Phase-split calculation. *Fluid phase equilibria*, **9**(1), 21–40.

Monroe, W., Silva, M., Larson, L. and Orr, F.J. [1990] Composition paths in four-component systems: effect of dissolved methane on 1D CO2 flood performance. *SPE Reservoir Engineering*, **5**(03), 423–432.

Orr, F.J. [2007] Theory of Gas Injection Processes - Tie-Line Publications.

Pires, A., Bedrikovetsky, P. and Shapiro, A. [2006] A splitting technique for analytical modelling of two-phase multicomponent flow in porous media. *Journal of Petroleum Science and Engineering*, **51**(1), 54–67.

Tang, D. and Zick, A. [1993] A new limited compositional reservoir simulator. In: *SPE Symposium on Reservoir Simulation*. Society of Petroleum Engineers.

Voskov, D. [2017] Operator-based linearization approach for modeling of multiphase multi-component flow in porous media. *Journal of Computational Physics*, **337**, 275–288.

Voskov, D. and Entov, V. [2001] Problem of oil displacement by gas mixtures. *Fluid Dynamics*, **36**(2), 269–278.
Voskov, D., Henley, H. and Lucia, A. [2017] Fully compositional multi-scale reservoir simulation of various CO2 sequestration mechanisms. *Computers and Chemical Engineering*, **96**, 183–195.
Voskov, D. and Tchelepi, H. [2008] Compositional space parametrization for miscible displacement simulation. *Transport in Porous Media*, **75**(1), 111–128.
Voskov, D. and Tchelepi, H. [2009a] Compositional space parameterization: Theory and Application for Immiscible Displacements. *SPE Journal*, **14**(03), 431–440.
Voskov, D. and Tchelepi, H. [2009b] Tie-simplex based mathematical framework for thermodynamical equilibrium computation of mixtures with an arbitrary number of phases. *Fluid Phase Equilibria*, **283**(1-2), 1–11.
Whitson, C. and Michelsen, M. [1989] The negative flash. *Fluid Phase Equilibria*, **53**, 51–71.
Zaydullin, R., Voskov, D. and Tchelepi, H. [2012] Nonlinear formulation based on an equation-of-state free method for compositional flow simulation. *SPE Journal*, **18**(02), 264–273.
Zhou, H., Lee, S. and Tchelepi, H. [2012] Multiscale finite-volume formulation for saturation equations. *SPE Journal*, **17**(01), 198–211.

Appendix A: Non tie-line rarefaction

The construction of a fractional flow solution curve is similar to the construction of a compositional path, which is generally represented by a set of shocks and rarefaction (both tie-line and non tie-line). Based on this underlying fact, the fractional flow solution curve (Frac.Sol curve in Fig. 11) is constructed in compliance with the conservation law. The cardinal difference between the traced solution curve that

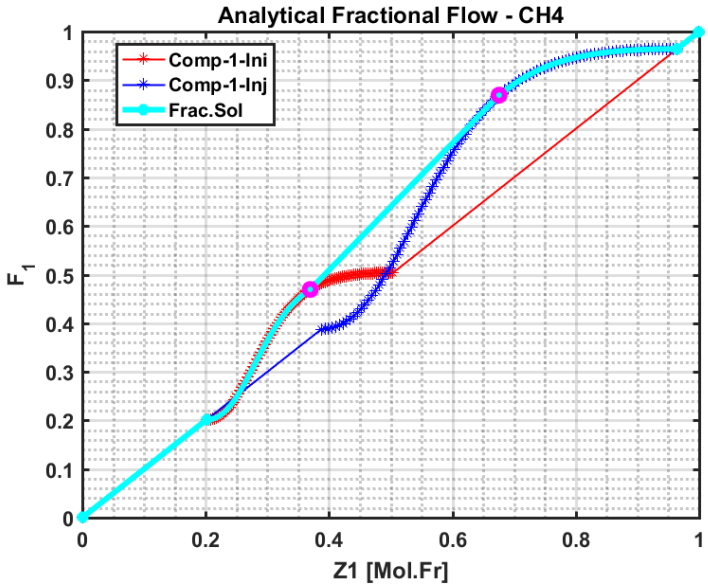


Figure 11 *Analytical fractional flow Curve based on non tie-line rarefaction.*

is implemented in the simulation and the one that is shown here is the path of non tie-line rarefaction (indicated by the straight line in between the pink dots). Though the traced solution curve indicated above ensures conservation, the locating of these points on the fractional flow 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 construct or trace the fractional flow s olution c urve w ith r espect t o t he shock regions). As a result, the solution profile within the two-phase region is sporadic.

Appendix B: Reconstruction of 5C system

The modified transport equation based on CSP technique is solved over the 3D parameterized space (as shown in Fig. 10) and the corresponding results of reconstruction are shown below in Fig. 12. By parameterizing the phase variables effectively in the γ space, the number of equations solved inside the newton loop is profoundly reduced from n_c-1 to 2 (σ and v), with still holding to the fine scale accuracy. Further, these results also reinstates the fact that the proposed CSP approach is extremely flexible in terms of implementation and applications, yielding to a coarse system representation and thereby enhancing the computational efficiency.

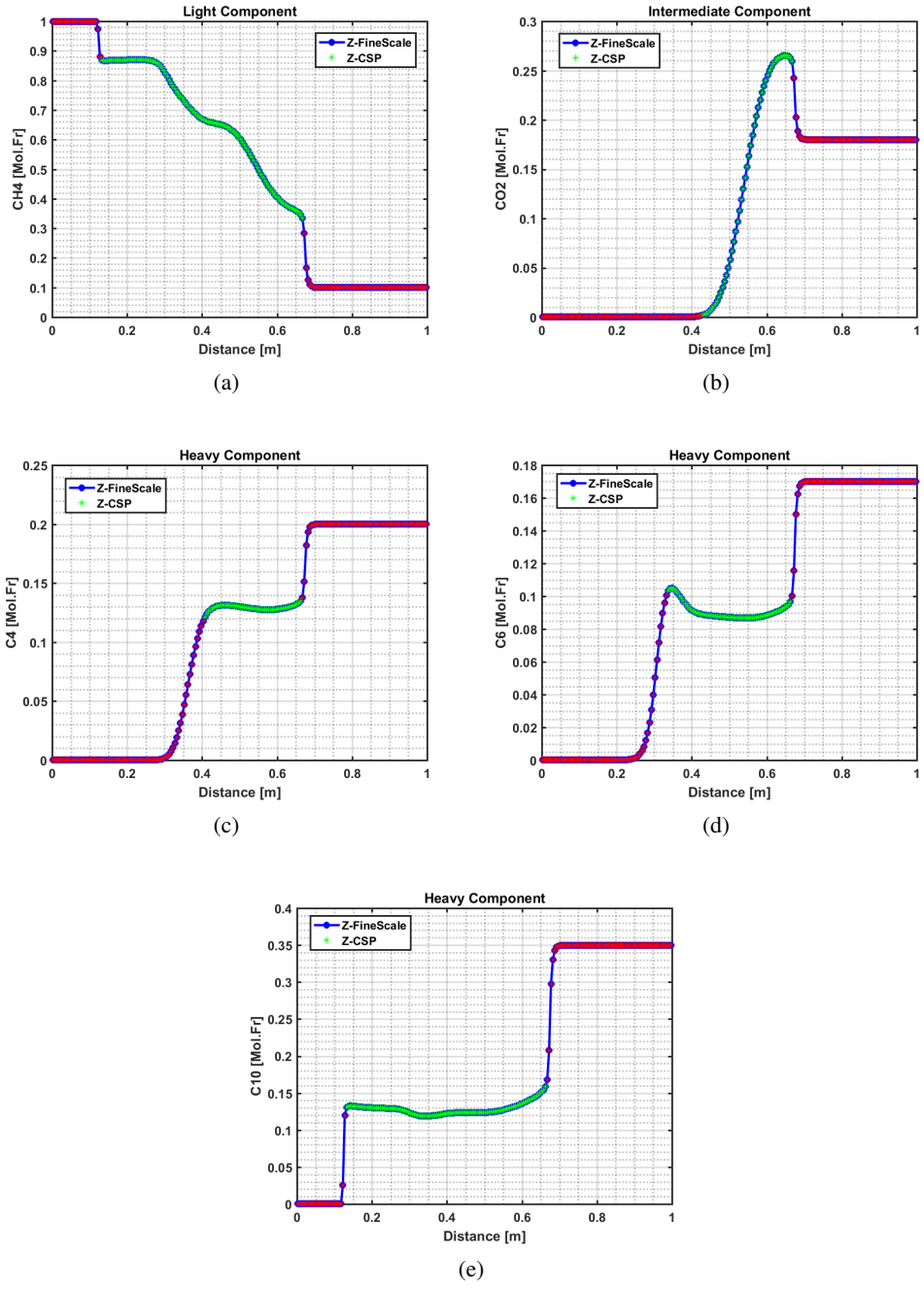


Figure 12 *Reconstructed 2-phase region of 5C system, vaporizing gas drive (a) Light Component-C_1 (b) Intermediate Component-CO_2 (c) Heavy Component-C_4 (d) Heavy Component-C_6 (e) Heavy Component-C_{10}.*

Appendix C: Initial and Injection compositions used in simulation

Table 2 and 3 shows the injection gas and initial oil composition used in the validation of *constant K-value* based system on the basis of proposed technique.

Table 2 *Quaternary system, constant K-values (vaporizing gas drive).*

	Quaternary system			
Compositions	C_1	CO_2	C_4	C_{10}
Initial Oil Compositions	0.10	0.18	0.37	0.35
Injection gas Compositions	0.97	0.01	0.01	0.01
K-values	2.5	1.5	0.5	0.05

For the vaporizing gas drive mechanism, a lean gas mixture primarily containing methane is injected to displace the oil composition (mixture of butane and decane). In a condensing gas drive mechanism, the injection gas composition is primarily enriched with the intermediate component. The compositions described here are selected based on the description given in (Orr, 2007).

Table 3 *Quaternary system, constant K-value (condensing gas drive).*

	Quaternary system			
Compositions	C_1	CO_2	C_4	C_{10}
Initial Oil Compositions	0.01	0.01	0.39	0.59
Injection gas Compositions	0.59	0.39	0.01	0.01
K-values	2.5	1.5	0.5	0.05

Table 4 and 5 shows the injection gas and initial oil composition used in the validation of *EoS* based system. Both binary and quaternary system has been simulated with injection gas - containing predominantly the intermediate component to displace the oil composition containing butane and decane.

Table 4 *Binary system (validation for EoS).*

	Binary system	
Compositions	CO_2	C_{10}
Initial Oil Compositions	0.33	0.67
Injection gas Compositions	0.997	0.003

Table 5 *Quaternary system (validation for Eos).*

	Quaternary system			
Compositions	CO_2	C_1	NC_4	C_{10}
Initial Oil Compositions	0.33	0.03	0.24	0.40
Injection gas Compositions	0.997	0.001	0.001	0.001