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Multiscale Reconstruction of Compositional Transport

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by

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Abstract

Designing strategies for efficient oil production from reservoirs rely heavily on reservoir simulation studies, which in-turn is based on various nonlinear formulations. It is therefore very important to develop a robust simulation model that captures the flow of various components present in different phases and the associated thermodynamic and chemical interactions. A compositional formulation is a reliable option for understanding these complex subsurface processes. However, this type of model has a great computational cost, since the number of equations (n_c) that needs to be solved in each grid block increases proportionally with the number of components employed.

The solution of the multicomponent multiphase flow problem is obtained by solving the associated nonlinear governing equation describing the conservation of mass, thereby determining the pressure (P) and compositional changes (Z) of the system. On the other hand, an Equation of state (EoS) model is employed to describe the phase behavior of the system, which in turn is accomplished in two stages: *phase stability test* - to identify the existence of number of phase in a particular grid cell and *flash calculation* - to determine the split fraction of components amongst the phases present. The aforesaid procedure is referred as the *standard EoS* based approach to solve compositional problem and they are generally arduous.

In previous works, a compositional-space parameterization 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 the two key tie-lines that extend through the initial and the 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 composition solution onto the full tie-line space is invariant to the hydrodynamic property of the compositional system.

Here we utilize this technique to develop a multiscale reconstruction of compositional transport. Two types of prolongation operators are defined based on the local saturation history, with each having different computational complexities. In the first stage, a fine scale prolongation operator is implemented on a modified conservation equation with the objective of reconstructing the leading and trailing shock positions in space. Once the position of shocks are identified, the solution lying in the regions outside the shock can be solved on a coarse-scale mesh, since the structure of the transport solution outside of the two-phase region is relatively simple. Later, the fine scale projection of this coarse solution is carried out using the constant prolongation operator. The solution for n_c components lying in between leading and trailing shocks is reconstructed by solving just two equations. The proposed reconstruction strategy results in coarsening of the compositional problem, both in space and representation. By this way, the simulation time is appreciably reduced by several folds without significant loss in accuracy of the results. Also, the proposed multiscale technique is evaluated by comparing them with a suitable upscaling methodology, since they are generally characterized by an affable framework of implementation and one of the most widely sought out ways to enhance computational efficiency.

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Nomenclature

Symbol	Description	Units
k	Absolute Permeability	Darcy
μ_g	Viscosity of gas	Pa.S
μ_o	Viscosity of oil	Pa.S
$ ho_g$	Density of gas	Kg/m^3
$ ho_o$	Density of oil	Kg/m^3
ϕ	Porosity	_
K _i	Equilibrium ratio of component i	_
ν	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	_
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
Р	Pressure	N/m^2
σ	Parameterized Variable	-
n_c	Number of components	-
n_p	Number of phases	_

Introduction

A coupled description of flow and compositional changes spans a wide range of length and timescales. The subsurface heterogeneity with complex multi-scale features introduce additional challenges. Hence we need appropriate and suitable methods which can solve these interactions occurring at the subsurface in a robust manner. A compositional model is a reliable option for understanding these complex subsurface processes and interactions. On the other, these simulations 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. It is also dangerous to compromise on the resolution of the numerical problem to speed up the computations, as they are dispersive in nature [19]. Being a vital tool for various oil recovery applications, the use of high resolution compositional simulations are ineluctable. Hence, there is a strong need to address the computational complexities associated with them, thus laying down the motivation for this research work.

The solution of the multicomponent multiphase flow problem is obtained by solving the associated nonlinear governing equation describing the conservation of mass. An equations of state (EoS) model is generally employed to describe the phase behavior of the system and they are generally computed in two stages: *phase stability test* [21] - to identify the existence of number of phase in a particular grid cell and *flash calculation* [22] - to determine the split fraction of components amongst the phases present. A nonlinear system of thermodynamic constraints is used to represent the instantaneous thermodynamic equilibrium of the mixture. The aforesaid procedure is also referred as the *standard EoS* based approach for phase behavior computation in compositional problem.

Significant progress have been made to enhance the performance of compositional simulators. Especially, several efforts were made to describe the entire system on the basis of pseudo-ternary representation [15] & [6] and such representations were found to be valid for general compositional problem [12]. In [12], it was proven as well that the solution route enters and exits the two phase region by a shock and that these shocks coincides with the tie-line and its extension. Later, an insightful demonstration on the basis of a unified *Method* of *Characteristics* (MOC) framework was carried out on a gas injection processes [29] & [27]. The theory was limited to 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 [13].

On the basis of these ideas, a general approach for solving a compositional problem with the assumption of constant partitioning coefficients was proposed [25]. This approach used the fact that the structure of solution in tie-line space is independent of any changes in hydrodynamic properties of the system. However, this fact was based on a general key tielines theory and was not appropriately proven. A numerical framework, describing similar ideology (based on the tie-line concept) was later implemented for a more general case [10] & [28], where the original compositional problem is projected onto a tie-line space, and later, the parameters pertaining to two-phase region of EoS-based system are determined using polynomial approximations.

Subsequently, further developments were made in determining the solution of the compositional problem in this 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 as the 'Compositional Space Parameterization' (CSP) [7]. Also, it was proven that the projection of solution to the tie-line space is invariant to the hydrodynamic parameters of the problem [3]. The CSP ideology eventually led to the development of Compositional Space Adaptive Tabulation (CSAT) method [7], 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. The proposed techniques not only accelerated the phase behavioral computations, but also provided the basis for development of fully EOS-free compositional simulation approach [26].

On the basis of these ideas, we are proposing here a multiscale reconstruction of the compositional transport problem. The solution of the problem is reconstructed at a fine scale accuracy without actually solving the full system of equations at fine scale. This multiscale technique is totally new as far as compositional simulation is concerned. The methodology has been tested for several multicomponent gas injection problems and has been found to be robust and efficient. An improved version of compositional space parametrization technique has been developed and successfully used in this study.

Alternatively, an Upscaling technique, which is generally the widely sought out strategy to enhance the computational efficiency was also tested and evaluated. An upscaling technique is generally characterized by an affable framework of implementation but at the same time, it is challenging to use them in a compositional flow problem due to the variations in phase compositions, as well as in saturation and velocities. On a broad perspective, these techniques are classified into the upscaling of single phase flow parameters (absolute permeability) [31] and multiphase flow functions (phase relative permeabilities) [30]. For a compositional transport problem, previous studies were generally based on use of transport coefficients, computed for each components and in each phases to capture the average fine scale fluxes [23] & [17]. Recently, a new approach, based on non-equilibrium thermodynamic representation at coarse scale, was proposed and tested [2]. The non-equilibrium behavior is modeled based on upscaled thermodynamic functions, which in turn is described based on the difference in component fugacities. In our work, we have demonstrated the implementation of two different averaging techniques to reconstruct the solution of transport problem. The primary objective of performing such implementation is to evaluate the performance of the proposed multiscale technique in comparison with the upscaling approach.

The report is organized as follows: Initially a brief overview about the compositional problem and the associated terminologies have been described, followed by insight on the standard EOS based simulation approach. The methodology describing the multiscale reconstruction strategy and upscaling methodology of a compositional problem is explained subsequently. 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.

\sum

Overview

2.1. Ternary Phase Diagram

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 a given thermodynamic conditions (pressure and temperature), the light component is present in gas phase and the heavy component is present in the 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) are directly driven by the compositional changes and it is generally represented on a phase diagram ¹. The *Fig. 2.1* represents the phase diagram of a ternary system (3 components) and it is also known as *ternary phase diagram*.



Figure 2.1: Ternary phase diagram representing a 3-component system, Source:Petrowiki

¹Phase diagrams are a graphical representation of different phase existing at various ranges of temperature and pressure within a reservoir

The *ternary diagram* is an equal sided triangle with unit height. The vertices's of the triangle represents a mixture of pure (100%) component (as labeled in the vertex) and the side across the vertex represents a binary system with the absence (zero fraction) of this particular component. For instance, the mole fraction of light component on the line connecting the intermediate and heavy component is zero. Also, any composition within the triangular space can be uniquely described on the basis of *level rule*, such that the sum of component fraction always adds to unity.

A *binodal curve* distinguishes the single phase compositions with those existing in two phases. The two phase compositions lies 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 in equilibrium by a *tie-line*. Both the binodal curve and the equilibrium tie-lines are strong functions of thermodynamic conditions (pressure & temperature). As the tie-line connects the compositions of liquid and vapor phases in equilibrium, any mixture with an overall composition along a single tie-line gives the same liquid and vapor compositions. Only the amounts of liquid and vapor changes as the overall composition changes from liquid side of the binodal curve to the vapor side.

The liquid and vapor phase compositions on the binodal curve meets at the *critical point* or the *plait point*, where both the liquid and vapor phases are identical. Also the length of the tie-line at this point is zero. For a given temperature and pressure, the critical point mixture is unique in a two-phase 3-component system.

2.2. Compositional Simulation Framework

The compositional simulation framework can be broadly separated into two sections, namely the *thermodynamic part* and the *hydrodynamic part*. The 'thermodynamic computations' enables us to determine the phase behavior of the system with the aid of phase stability test and flash calculation and the 'hydrodynamic computations' attribute to the solution of flow and transport equations, thereby determining the pressure and the compositional changes of the system. Both these computations are strongly coupled with each other and a comprehensive explanation on the same, along with the supporting equations are given in section (2.2.1) & (2.2.2).

2.2.1. Thermodynamic Computations

The primary objective of solving the thermodynamic system of equation is to understand the phase behavior of the system and to determine the associated parameters like the number of physically existing phases, phase fractions, etc. These computations are carried out in two stages as described below:

- Phase Stability Test
- Flash Calculation

Both these tests involves different computational complexities. The usage and implementation aspect of the described two stages are discussed below in detail.

Phase Stability Test

The main purpose of phase stability analysis is to determine the number of equilibrium phases that exist in a multicomponent system. The conventional approach of performing the stability analysis is based on an initial assumption of the number of phases present and subsequent determination of the stable condition with the minimum Gibbs energy [11]. In the modern reservoir simulation, a stability test based on *Tangent Plane Distance* (TPD) criteria [21] is used in numerical implementations.

The Gibbs energy of a mixture is define based on the following equation:

$$G_o = \sum_{i=1}^{n_c} n_i \mu_i^o,$$
 (2.1)

where n_i is the component mole fraction and μ_i^o is the chemical potential. If the mixture is divided into two phases (phase I & phase II), say with mole numbers $N - \psi'$ and ψ' , then the change in the Gibbs free energy is given by:

$$\Delta G = G(N - \psi) + G(\psi) - G_o \tag{2.2}$$

On applying Taylor series expansion on equ (2.2), the change in the Gibbs energy is reduced to the form:

$$F(y) = \sum_{i=1}^{n_c} y_i \left(\mu_i(y) - (\mu_i^o) \right) \ge 0$$
(2.3)

where y is the mole fraction in phase II. The equ. (2.3) is also referred as the stability condition for determining the number of existing equilibrium phases in the system. In other words, the stability of the single phase state requires that its Gibbs energy is at a global minimum with any trial compositions. The TPD criterion described in [21], explains how to choose a sufficient number of such trial compositions in a two-phase multicomponent system.

Flash Calculation

Once the phase stability test identifies the number of physically existing phases in the system, the flash calculation is subsequently performed to determine the partitioning of components amongst these phases. The flash calculation can be carried out either based on *equilibrium* ratios (also known as K values - defined as the ratio of phase equilibrium fractions $K_i = y_i/x_i$) 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, as it just chosen for simplicity.

It is also worth noticing that, in a general hydrocarbon system, the K-values can be a strong function of composition (especially at higher pressures). In this work, we assume a low pressure system involving an immiscible displacement process without the critical region. Under these conditions, it is quite reasonable to assume a constant K-values without compositional dependency. Hence, the same has been implemented in the simulation framework.

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

$$h(v) = \sum_{i=1}^{n_c} \left[\frac{Z_i(K_i - 1)}{v(K_i - 1) + 1} \right] = 0.$$
(2.4)

The nonlinear equ. (2.4) is also referred as the Rachford-Rice equation [4], which can be solved by Newton-Raphson technique to determine the vapor phase fraction (v). The convergence of the above equation is achieved if the resulting vapor phase fraction lies in the range (1/(1- K_{max}) < $v < 1/(1-K_{min})$), where K_{max} and K_{min} refers to the largest and smallest K-values of the system. In other words, the solution of Rachford-Rice equation is bounded by two asymptotes defined by the K-values of the system (refer *Fig. 2.2* for example).

Once the value of 'v' have been determined, the corresponding phase compositions are computed based on equ. (2.5)-(2.6) as shown below:

$$x_i = \frac{Z_i}{(\nu(K_i - 1) + 1)}$$
(2.5)

$$y_i = K_i x_i \tag{2.6}$$



Figure 2.2: Asymptotic solution of Rachford-Rice equation for three component system

It is also worth noticing the fact that, the concept of flash calculation is not limited to twophase mixtures alone as they can also be performed on single phase compositions [4]. Such a phase computation is generally referred as the *negative-flash calculation*, where the equ. (2.4) is solved for the vapor phase fraction (v) of single phase compositions. The resulting value will either be less than zero (v<0) if liquid phase is present, or greater than one (v>1) if vapor phase is present. The phase stability test (equ. 2.3) becomes obsolete in this approach since a single negative-flash procedure (equ. 2.4) can predict both the phase stability and phase split of the existing compositions.

The idea behind the negative flash calculation is that a single phase mixture is present as a linear combination of phase composition and they always lies on the extension of the tielines. It is worth noticing that the we have adopted the negative flash based framework to determine the phase behavior of the system.

2.2.2. Hydrodynamic Computations

The underlying principle that governs the hydrodynamic computations is the conservation of mass, which is generally defined over an arbitrary volume as stated below,

$$\underbrace{Mass \ Final - Mass \ Initial}_{Accumulation} = \underbrace{Mass \ In - Mass \ Out}_{Net \ Flux \ In} + \underbrace{Generation}_{Source}$$
(2.7)

By expressing this ideology in a continuous form, we arrive at the transport equation describing a physical phenomenon. For an isothermal compositional system consisting of n_c components and 2 hydrocarbon phases [26], the transport equation is given by:

$$\frac{\partial}{\partial t}\phi\left[(x_i\rho_oS_o) + (y_i\rho_gS_g)\right] + \nabla \cdot \left[(x_i\overline{u_o}\rho_o) + (y_i\overline{u_g}\rho_g)\right] + \left[(x_i\rho_oq_o) + (y_i\rho_gq_g)\right] = 0, \ i = 1, \dots, n_c \quad (2.8)$$

where, ϕ is the porosity, $S_g \& S_o$ are the saturation of gas and oil phase, $\rho_g \& \rho_o$ are the molar density of gas and oil phase, $x_i \& y_i$ are the liquid and vapor molar fraction of component 'i', $u_g \& u_o$ are the Darcy velocity of gas and oil phase and n_c indicates the total number of discrete components present in the system. Note that the equ. (2.8) is valid for a system with the absence of capillarity, diffusion and chemical reactions. The velocity of the fluid phases are usually described based on Darcy's law as shown in equ. (2.9):

$$\overline{u_j} = -\overline{\overline{K}} \frac{k_{rj}}{\mu_j} \nabla P, \quad j = 1, 2$$
(2.9)

where, \overline{K} is the absolute permeability, $k_{r,j}$ is the relative permeability of phase 'j', μ_j is the phase viscosity. The phase mobility (λ_j) is defined as the ratio of $k_{r,j}/\mu_j$, where the relative permeabilities are functions of saturation.

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 [9], refer equ. (2.10) below.

$$f_{i,g}(P,T,y_i) = f_{i,o}(P,T,x_i)$$
 (2.10)

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). Finally, the auxiliary relations used in closing the system of equations are given by equ. (2.11)-(2.12):

$$\sum_{i=1}^{n_c} x_i - 1 = 0 \quad \& \quad \sum_{i=1}^{n_c} y_i - 1 = 0$$
(2.11)

$$S_o + S_g = 1$$
 (2.12)

The system of equ. (2.8)-(2.12) is generally referred as the standard EoS-based formulation of a compositional problem.

For a one-dimensional reservoir, under the assumption of incompressible flow regime with equal densities and absence of source term, the governing transport equation [7] can be further simplified as:

$$\frac{\partial Z_i}{\partial t} + \frac{U_t}{\phi} \frac{\partial F_i}{\partial x} = 0, \quad i = 1, \dots, n_c$$
(2.13)

where,

$$Z_i = x_i(1-v) + y_i v (2.14)$$

and

$$(x_i u_o + y_i u_g) = U_t F_i \tag{2.15}$$

$$:: [(x_i u_o + y_i u_g) = U_t (x_i (1 - f_g) + y_i f_g) \& F_i = x_i (1 - f_g) + y_i f_g]$$

The simplified form of the transport equ. (2.13) is eventually discretized and solved numerically to determine the full solution (overall composition - Z_i). As the main focus of this research is solely devoted on improving the performance of the transport solver, a standard sequential strategy has been followed to compute the pressure and velocity of the system by solving the flow equation.

2.3. Nonlinear Formulations

The convolution of the compositional problem is associated with the nonlinear coupling of thermodynamics - which describes the partitioning of components amongst the two phases, with the transport of multiple components. A wide range of simulation frameworks have been proposed [18] in terms of various nonlinear formulations to solve this highly coupled system of equations. Based on this approach, the full coupled system of the compositional problem is reduced into a definite number of primary equations and primary unknowns. Later, these primary variables are used along with the secondary equations to solve for the remaining secondary unknowns.

The critical aspect of this technique lies in the choice of dividing the equations and unknowns into primary and secondary sets. These choices lead to a whole set of varied formulations [9] out of which the most widely used are the natural variable formulation [20] and the molar variable formulation [14] & [5].

In this research work, the molar variable formulation has been implemented in the simulation framework. Based on this formulation, the choice of primary variables are as shown below:

- Pressure (P) [1]
- Overall Composition $(Z_i) [n_c 1]$

The transport equ. (2.13) is used as the primary equation to solve for primary unknowns. An *explicit* scheme is adopted to solve this PDE numerically and the discretized form of the same is given by:

$$Z_{n+1} = Z_n - \frac{dt}{\phi \cdot dx} \left\{ (F_i \cdot U_{i+1}) - (F_{i-1} \cdot U_i) \right\}_n \quad i = 1, \dots, n_c - 1$$
(2.16)

The explicit method calculates the compositional changes of the system at the current time on the basis of compositions from the previous time step. We also have to be mindful about the size of the timestep since this approach is conditionally stable. The stability criterion is defined based on the *CFL* condition, which defines the size of the time step to march on. The residual form of the discretized conservation equ. (2.16) can be written as:

$$R = Z_{n+1} - Z_n - \frac{dt}{\phi \cdot dx} \left\{ (F_i \cdot U_{i+1}) - (F_{i-1} \cdot U_i) \right\}_n \quad i = 1, \dots, n_c - 1$$
(2.17)

Once the primary variables are determined, they are substituted in the secondary equations to determine the solution for secondary unknowns. For instance, the phase compositions are obtained based on equ. (2.5)-(2.6). The phase saturation is determined based on the equ. (2.18) as shown below:

$$S_g = \frac{\frac{\overline{\rho_g}}{\overline{\rho_g}}}{\frac{v}{\rho_g} + \frac{(1-v)}{\rho_o}}$$
(2.18)

where, $S_g \& S_o$ represents the saturation of gas and oil phase, $\rho_g \& \rho_o$ are the densities of gas and oil phase, v is the vapor phase fraction. The phase densities are generally computed based on equations of state, but in this case they are assumed to be constant as the flow regime is incompressible. To simplify the derivations, we also assume that the density of phases are constant and equal to each other.

2.4. General Structure of Compositional Solution

The solution of a compositional problem for gas injection process can be predominantly described in a phase diagram, analogous to description of a trajectory in compositional space. This 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 governs the construction of the solution (compositional path) is the *conservation* and *entropy* conditions, resulting in a series of self-sharpening waves (shocks) and spreading waves (rarefaction) as shown in *Fig. 2.3*. These changes are generally consistent with the above mentioned physical principles.

The fractional flow theory gives an insight on fluid mobility in the presence of other fluid phases. *Fig. 2.3(a)* shows a plot of fractional flow as a function of composition. The velocity of each composition in this plot follows a simple rule - where 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 in the system [29] & [27]. These two shocks are referred to as the *leading shock* and the *trailing shock*.



Figure 2.3: General structure of compositional solution (a) Fractional flow curve (b) Solution profile-Light Component (c) Ternary phase diagram

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 depend 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.

Further insight on the shock solution is described based on the Rankine-Hugoniot condition [12], which is given by the equ. (2.19) [13]:

$$\Lambda = \frac{dF_i}{dZ_i} = \frac{F_{i,2} - F_{i,1}}{Z_{i,2} - Z_{i,1}} \quad i = 1, \dots, n_c$$
(2.19)

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-Hugoniot condition is an integral version of the conservation equation shown in equ. (2.13) and it illustrates the fact that the volume is conserved across the shock.

Unlike a binary displacement problem, where the compositional changes driven by trailing and leading shocks occurs over a single tie-line (due to Gibbs degrees of freedom), in a three or more component systems, the compositional changes occurs along injection and initial tie-lines (referred as a tie-line rarefaction, shown in *Fig. 2.3(c)*) as well as between tie-lines (referred as a non tie-line rarefaction, shown in *Fig. 2.3(c)*). All those tie-lines involved in the construction of compositional path are referred as the key tie-lines of the system.

The aforesaid concept are always valid and holds good irrespective of the number of components present in the system. As we consider a system with more than three components, there are some subtle variations in the construction of the compositional path, thereby leading to changes in their representation in the phase diagram. For example, the solution of a four component system is generally represented on an quaternary diagram based on equilateral tetrahedron, refer *Fig. 2.4* below.



Figure 2.4: Quaternary phase diagram representing a 4-component system [7]

Each face of the quaternary diagram represents a ternary system and the band across these faces (or) the interior of the diagram represents a two-phase region. Unlike a ternary system, where two key tie-lines lie in the same plane, here they lie in different planes and a third key tie-line, known as the *crossover tie-line*, is used to construct the solution from the initial oil composition to injection gas composition.

3

Methodology

3.1. Motivation

Recently, the multiscale techniques have been widely explored and researched in order to develop computationally efficient simulation. In this approach, the solution of the complex reservoir problems are determined in full resolution (fine scale) by using the solution of reduced system of equations [24]. With the advent of these techniques, the performance of the flow solvers (pressure & total velocity) have been significantly improved whilst the transport problem is still continued to be solved at fine scale resolution. As a result, the simulation processes continues to remain cumbersome.

With the objective of speeding up the computations pertaining to transport solver, an adaptive *Multiscale Finite Volume* (MSFV) approach was proposed in [16]. Based on this technique, the transport problem is initially solved on a coarse scale and later the results are constructed at fine scale with the use of *adaptive prolongation operators*. Three multiscale operators are defined (FVFS,AVFS, AS)¹ and used during the coarse of simulation, with each having different computational complexities. The basis of these prolongation operators are the local saturation history of the system. This methodology was implemented on a *Buckley-Leverett* problem [16] and the results were found to be accurate with the reference fine scale solution. On the basis of this insightful methodology, we are herewith proposing a robust technique for reconstructing the solution of compositional transport problem with arbitrary number of components.

3.2. Numerical Framework

In this research work, the optimization of the compositional transport problem is carried out on two different frameworks as described below, with distinctive computational features.

- Multiscale Reconstruction
- Upscaling (Coarse Scale Reconstruction)

The multiscale framework constitute of a two stage simulation strategy through which the solution of the transport problem is reconstructed in an optimized way. On the other hand, the upscaling framework is based on classical averaging techniques, thereby resulting in a coarse (in space) solution of the transport problem. Both these approaches are efficient and involve simple and straight forward implementation. The primary objective of carrying out the reconstruction on two different frameworks is to evaluate their performance against one another before drawing conclusions.

¹FVFS-Full Velocity and Full Saturation, AVFS-Approximate Velocity and Full Saturation, AS-Approximate Saturation

3.3. Reconstruction of Transport Problem - Multiscale

3.3.1. Overview

The inception of the multiscale based reconstruction technique is attributed to the saturation history of the compositional problem. *Fig. 3.1* shows the saturation plot of a gas injection process. Here, the saturation profile can be classified into *three* distinctive regions, based on the characteristic changes of saturation. The *region 1* corresponds to a placid zone, where the gas saturation values remains (almost) constant. The *region 2* corresponds to shock solution, where there is a pronounced jump (shock) in the saturation values. The characteristics of this shock solutions are defined based on the Rankine-Hugoniot condition (equ. 2.19). Finally, the *region 3* refers to a fan characteristics (rarefaction) where the saturation changes are more continuous. The region 1 and region 3 are also referred as "single phase region" and "two phase region" respectively, while region 2 is a "transition zone".



Figure 3.1: Gas saturation plot of a quaternary system, Vaporizing gas drive

On the basis of this classification, it can be observed 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 apprehending fact lays down the basis of the proposed multiscale technique, where specially constructed prolongation operators and parameterization techniques are implemented on the different regions of saturations, thereby reconstructing the solution for the entire problem.

Initially, we reconstruct the position of shock in space as they hold the key for this reconstruction and the same is being carried out using an fine scale prolongation operator - "A2F". Once the shocks position are identified, the solution of the two phase region (lying in between the shocks) is reconstructed based on 'Compositional Space Parameterization' (CSP) technique with reduced system of equations. Subsequently, the solution for the regions lying outside the shocks are determined by solving the conservation equation on coarser scale since the solution for this region (single phase) is relatively simple and straight forward as there is seldom change in their compositions. Later, they are projected onto fine scale using an constant prolongation operator - "AS" [16]. This way, the solution of the entire transport problem is effectively reconstructed in a multiscale framework without significant loss in accuracy. Also the proposed reconstruction strategy results in coarsening of the compositional transport problem in terms of space (grid resolutions) as well as the system representation (number of equations), thereby enhancing the computational efficiency.

3.3.2. Multiscale Reconstruction of Shocks

The multiscale reconstruction of the shock solution is based on the concept of fractional flow, where we analytically construct the special fractional flow curve based on the tie-lines passing through the injection and initial composition. Subsequently, an equivalent solution is constructed for one component based on this specially constructed analytical curve by tracing the position of leading and trailing shocks, refer *Fig. 3.2* for example.



Figure 3.2: Analytical fractional flow Curve of Light Component-CH4

Initially, 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. Now by keeping this ' x_i ' and ' y_i ' values constant, the fractional flow curve is analytically constructed in the 2-phase region based on equ. (3.1) [10].

$$F_i = x_i(1 - f_a) + y_i f_a, \quad i = 1, \dots, (n_c - 1)$$
(3.1)

The fractional flow plot is an S-shaped curve within the two phase region (*Fig. 3.2*). In the single phase region, 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 as shown in *Fig. 3.3*. By this way, the fractional curves are analytically constructed on the injection and initial tie-line of the system.

Once these curves are constructed, they are eventually plotted together and a multiscale fractional flow curve is constructed by tracing these two curves from injection to initial composition. The tracing is done in such a way that the switch between the initial and injection curves occurs at the point of intersection (can also be viewed as a substitute for a non tie-line path). The constructed curve, shown in *Fig. 3.2 & Fig. 3.3* as *Frac.Sol*, represents the equivalent solution of F_i' for the corresponding Z_i' . Later these values are tabulated and defined as a prolongation operator ('A2F') during the coarse of simulation, in order to determine the shock positions in space.



Figure 3.3: Analytical fractional flow curve (a) C-10 component and (b) C-4 component

3.3.3. Multiscale Reconstruction of 2-Phase Region

Compositional Space Parameterization (CSP)

The part of the solution, belonging to the two-phase region, is reconstructed based on *tie-line* parameterization technique. This approach is based on the fact that the phase behavior of an gas-injection processes is predominantly controlled by $(n_c - 1)$ key tie-lines and hence it is convenient to parameterize the problem based on them.

On considering a system of n_c components, the overall mole fraction of any component Z_i in the mixture is defined by the equ. (3.2) [7].

$$Z_i = y_i v + x_i (1 - v), \quad i = 1, ..., (n_c - 1)$$
(3.2)

Along the tie-line or its extension it is also possible to represent the overall mole fraction of any component Z_i as a linear function of *one component* concentration and *tie-line parameters* [10], refer equ. (3.3)-(3.4) [7].

$$v = \frac{Z_1 - y_1}{x_1 - y_1} \tag{3.3}$$

Substituting equ. (3.3) in (3.2), we get:

$$Z_i = Z_1 \frac{x_i - y_i}{x_1 - y_1} + (y_i - y_1) \frac{x_i - y_i}{x_1 - y_1}, \quad i = 1, \dots, (n_c - 1)$$
(3.4)

Now, these phase variables (liquid and the vapor fractions) shown in equ. (3.4) are parameterized by a variable termed - " γ ", described on the basis of structure and properties of the tie-lines. By this way, each tie-line is uniquely characterized by a ' γ ' value. It is also worth noticing that the parameterizing variable (γ) can be defined arbitrarily in the compositional space except for the fact that the tie-lines should be able to be located uniquely. For instance, they can be defined as a tie-line trace on the face of compositional diagram [10], (or) at a plane representing the tie-line centers [7]. Once these variables are defined, we can plot the projection of full solution to a tie-line space (γ -path). Fig. 3.4 shows the solution in tie-line space of a 4-component system.



Figure 3.4: Parameterized space (*γ*-path)

The 'x' (γ_1) and 'y' (γ_2) axis in *Fig. 3.4* refers to the phase fractions of component-2 and component-3 in a four component system. An analogous illustration to the γ -path (in the tie-line space) is generally given by a simple projection of the compositional path on to a single plane. In a four component system, the ' γ '-path (*Fig. 3.4*) is viewed in the phase diagram as shown in *Fig. 3.5*.



Figure 3.5: Projection of compositional path onto a single plane [7]

Eventually, the relation describing the overall mole fraction (Z_i) is rewritten in the parameterized form as shown in equ. (3.5).

$$Z_i = A_i(\gamma)Z_1 + B_i(\gamma), \tag{3.5}$$

where,

$$A_{i} = \frac{x_{i} - y_{i}}{x_{1} - y_{1}}, \quad B_{i} = (y_{i} - y_{1})\frac{x_{i} - y_{i}}{x_{1} - y_{1}}$$
(3.6)

Here, the parameters A_i and B_i (shown in equ. 3.5) are constant for a given tie-line in the two phase region or its extension and changes only with the change in tie-lines [7].

Once the parameterized space representing the tie-line variables are established, the compositional transport problem is solved in this parameterized space to compute the compositional changes (Z_i) and this methodology is referred as the 'Compositional Space Parameterization' technique [10]. The transport problem (equ. 2.13) is also reformulated based on the CSP technique and it takes the following form:

$$\frac{\partial Z_1}{\partial t} + \frac{U_t}{\phi} \frac{\partial F_1}{\partial x} = 0, \tag{3.7}$$

$$\frac{\partial A_i Z_1 + B_i}{\partial t} + \frac{U_t}{\phi} \frac{\partial A_i F_1 + B_i}{\partial x} = 0 \quad i = 2, \dots, n_c - 1$$
(3.8)

The equ. (3.7)-(3.8) can be solved based on a splitting procedure [10]&[3] by formulating an equivalent auxiliary equation which in turn takes the form:

$$\frac{\partial A_i(\gamma)}{\partial \overline{\phi}} + \frac{\partial B_i(\gamma)}{\partial \overline{\psi}} = 0, \tag{3.9}$$

where $\overline{\phi} \& \overline{\psi}$ are the potential functions: $\overline{\phi}$ is equal to the volume of any component 'i' flowing across a control volume or trajectory and $\overline{\psi}$ ' refers to the flowing volume of overall composition. It is actually the conservative nature of equ. (3.7), which enables to make such representations in terms of potential functions. This auxiliary system of equ. (3.9) is also referred to as the *thermodynamic problem* of a compositional simulation [10]. It is also worth noticing that, the solution of the system (3.7)-(3.8), when projected in γ -space is equivalent to the solution of an auxiliary problem shown in equ. (3.9) [3].

The solution framework based on the splitting technique offers an subtle advantage to the CSP technique, thereby enhancing its effectiveness. It is based on the fact that the auxiliary system (thermodynamic problem) shown in equ. (3.9) contains only the phase behavior parameters, while the full problem shown in equ. (3.7)-(3.8) contains the thermodynamic parameters as well as the hydrodynamic properties. As a result, the solution of the thermodynamic problem (equ. 3.9) is totally *independent* of hydrodynamic characteristics [3]. In other words, irrespective of the changes associated with the flow parameters, like absolute or relative permeabilities, the decoupling effect of the thermodynamic problem provides an *invariant* γ -path (appendix A.3).

Solution of Hydrodynamic Problem

On the basis of the parameterization technique (CSP), an advanced simulation framework has been developed to solve the hydrodynamic problem and thereby reconstructing the solution of two phase region. Initially, the existing tie-lines of the system are parameterized based on γ' variables. Later they are projected on to a tie-line space resulting in a γ -path as shown in *Fig. 3.6.* The regions near the extreme end of the γ -path corresponds to the compositions lying on the injection and the initial tie-lines. The region where the slope of the γ -path changes drastically represents the compositions on the cross over tie-line. The γ -path in *Fig. 3.6* is an illustration for a four component system, where γ_1 and γ_2 indicated in the 'x' and 'y' axis refers to the phase fractions of intermediate components (components 2 and 3).

Once the γ -path is constructed, a new variable ' σ ', which is in turn described by a linear relationship between the end points of the γ -path, is introduced in the tie-line space. 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. 3.6*). By this way, the compositional variation of the entire problem is parameterized in tie-line space.

Now the solution for the two phase region (area within the leading and trailing shock) is determined by solving the transport problem in the parameterized space. The modified conservation equation (in residual form) solved in the CSP domain takes the form:

$$R_{i} = y_{i}(\sigma_{n+1}) \cdot v_{n+1} + x_{i}(\sigma_{n+1}) \cdot (1 - v_{n+1}) - Z_{n} - \frac{dt}{\phi \cdot dx} \left\{ (F_{i} \cdot U_{i+1}) - (F_{i-1} \cdot U_{i}) \right\}_{n} \quad i = 1, 2 \quad (3.10)$$



Figure 3.6: Parameterized space (γ -path) (a) Vaporizing gas drive (b) Condensing gas drive

Here, the tie-line parameters (' x_i ' & ' y_i ') (as shown in equ. 3.10) are functions of the parameterized variable ' σ '. The modified residual form (equ. 3.10) of the mass conservation equation is formulated by substituting the expression for overall mole fraction (equ. 3.2) in the residual form of the global problem (equ. 2.17). Also in the CSP domain, the n_c -1 primary variables of the global problem is replaced by just two primary variables (σ and v). In other words, the equ. (3.10) is solved with ' σ ' (parameterized variable) and 'v' (vapor fraction) as its primary unknowns instead of directly solving for the compositional changes (Z_i), thereby resulting in the coarsening of system's representation.

While solving the modified conservation equation (the residual form) in the tie-line space, it is imperative to be watchful of the fact that the relation (equ. 3.10) is nonlinear in nature, though the residual form (2.17) of the same problem is linear at global level. The nonlinearity here is induced by the tie-line parameters ($x_i \& y_i$) which is resolved using Newton-Raphson iterations based on primary variables (v and σ). In explicit framework used in this study, the introduced nonlinearities are local and it is resolved by a local nonlinear solution. In an implicit framework, these nonlinearities can be resolved within the same nonlinear loop, that is used in resolving the Fully Implicit approximation. The final system of relations (in algebraic form) is given by equ. (3.11).

$$J \cdot \begin{bmatrix} \delta v & \delta \sigma \end{bmatrix}^T = -\begin{bmatrix} R_1 & R_2 \end{bmatrix}^T$$
(3.11)

The residual (R) of the system is computed based on equ. (3.10) and the Jacobian (J) of the non linear system is determined by differentiating the residual (equ. 3.10) with respect to the unknown variables (v and σ). It is defined by a square matrix of size (2x2) as described in equ. (3.12)-(3.14).

$$J = \begin{bmatrix} \frac{\partial R_i}{\partial v} & \frac{\partial R_i}{\partial \sigma} \end{bmatrix} \quad i = 1, 2,$$
(3.12)

where

$$\frac{\partial R_i}{\partial v} = \{y_i(\sigma_{n+1}) - x_i(\sigma_{n+1})\} \quad i = 1, 2,$$
(3.13)

and

$$\frac{\partial R_i}{\partial \sigma} = \left\{ \left(\frac{\partial x_i}{\partial \sigma} \right)_{n+1} \cdot (1 - v_{n+1}) + \left(\frac{\partial y_i}{\partial \sigma} \right)_{n+1} \cdot (v_{n+1}) \right\} \quad i = 1, 2.$$
(3.14)

Once the solution for the primary variables are determined, the corresponding compositional changes (Z_i) are eventually computed in *two* stages. Initially the molar phase fractions (x_i) and y_i of n_c components are determined based on linear interpolation in the tie-line space, by using the solution of parameterized variable (σ) . In the second step, these interpolated phase behavior parameters are substituted in the secondary equ. (3.2) to determine the compositional changes (Z_i) . By this way, the solution of n_c components in the two phase region is effectively reconstructed by solving just *two* equations instead of n_c -1.

The performance evaluation of the described two stage reconstruction strategy, on the basis of multiscale approach is described in section (4.1.1) & (4.1.2) of the report.

3.4. Reconstruction of Transport Problem - Upscaling

An alternative approach based on upscaling methodology is implemented to reconstruct the solution of transport problem. The upscaling process is generally defined as an averaging procedure by which the static and the dynamic characteristics of a fine-scale model is approximated, resulting in a coarse-scale model. Here, we implemented two different averaging techniques to reconstruct solution at coarse scale. Unlike the multiscale approach, where the solution is reconstructed in two stages, here the entire solution is reconstructed in a single stage computation framework.

3.4.1. Volume Averaging

This averaging procedure is based on the overall composition at fine scale. Initially, a suitable upscaling / coarsening ratio is selected to define the resolution of the coarse scale problem. Later, the equ. (3.15) describing the concept of *volume averaging* is solved to determine the coarsened solution.

$$\langle Z_j \rangle = \frac{\sum Z_i V_i}{\sum V_i} \tag{3.15}$$

Here, z_j is the averaged compositional changes and V_i is the volume of the corresponding grid cells.

3.4.2. Compositional Averaging

Similar to the classic volume averaging technique, initially a suitable coarsening ratio is selected to define the coarse scale resolution. But unlike the previous case, here the quantity that is being averaged out is the molar volume [2] of each component and the corresponding phases present, refer equ. (3.16)-(3.18).

$$\overline{n_{i,g}} = \sum_{B_g} PV \rho_g Z_i + \sum_{B_{og}} PV S_g \rho_g y_i$$
(3.16)

$$\overline{n_{i,o}} = \sum_{B_o} PV \rho_o Z_i + \sum_{B_{og}} PV(1 - S_g) \rho_o x_i$$
(3.17)

$$\overline{n_{tot,g}} = \sum_{i=1}^{n_c} \overline{n_{i,g}} \quad \& \quad \overline{n_{tot,o}} = \sum_{i=1}^{n_c} \overline{n_{i,o}}$$
(3.18)

Once, the averaged quantities of the molar volume have been determined, they are subsequently substituted in equ. (3.19) to determine the upscaled solution of compositional changes $(\overline{Z_i})$.

$$\overline{Z_i} = \frac{\overline{n_{i,g}} + \overline{n_{i,o}}}{\overline{n_{tot,g}} + \overline{n_{tot,o}}}$$
(3.19)

On the other hand, the upscaled quantities attributing to the thermodynamic variables of the system are computed based on equ. (3.20)-(3.21).

$$\overline{y_i} = \frac{\overline{n_{i,g}}}{\overline{n_{tot,g}}} \quad \& \quad \overline{x_i} = \frac{\overline{n_{i,o}}}{\overline{n_{tot,o}}}$$
(3.20)

$$\overline{v_g} = \frac{\overline{n_{tot,g}}}{\overline{n_{tot,g}} + \overline{n_{tot,o}}}$$
(3.21)

Once the results are obtained based on the upscaling framework, they are eventually plotted in tandem with the global fine scale solution and studied for the accuracy (discussed in section 4.2).

4

Results & Discussion

In this section, we describe the results of reconstruction of the compositional transport problem, obtained based on *multiscale* and *upscaled* framework. The efficiency and robustness of the proposed methodology is investigated on a nonlinear transport equation describing *gas injection process*. For simplicity, we limit our implementation to 1D simulation which is not a limitation of the proposed technique. Both vaporizing and the condensing gas drive mechanisms have been modeled and studied in terms of accuracy. The injection and the initial compositions, used in the modeling of multicomponent system, are specified in appendix A.1. The hydrodynamic parameters used in the simulation are given in the Table. 4.1 below.

0.0
0.0
1.0
0.0
2.0
2.0
0.3
5.0
1.0

Table 4.1: Reservoir fluid properties

4.1. Reconstruction of Transport Problem - Multiscale

4.1.1. Reconstructed Shock Solution

The accurate determination of the shock position (leading and trailing shock) is of paramount importance in the proposed methodology. We reconstruct shock positions in space based on a multiscale framework, by using the A2F operator. A modified simulation strategy in accordance with the prolongation operator has been developed to construct the solution. The sequence of computations involved in this modified framework is similar to a standard sequential technique used in multiscale simulation. The only exception is that now the flow equation is solved along with a special transport equation based on prolongation operator (A2F).

The illustration of shock reconstruction is started by using a binary system. The *Fig. 4.1(a)* & *(b)* shows the analytical fractional flow and *Fig. 4.1 (c)* & *(d)* shows the reconstructed results, compared with the global fine scale solution.



Figure 4.1: Reconstructed full solution of binary system, Vaporising gas drive (a) Fractional flow of Light Component-CH4 (b) Fractional flow of Heavy Component-C10 (c) Full solution of Light Component-CH4 (d) Full solution of Heavy Component-C10

In a binary system (2 components), the entire compositional displacement occurs along a single tie-line (due to Gibbs phase rule). Hence, the fractional flow is just a single curve, as both the injection and the initial compositions lie on the same tie-line. Hence, the description of A2F operator is straight forward, as the tracing of curves described in section (3.3.2) is not

applicable here. Likewise, the shock reconstruction framework (using A2F operator) alone is sufficient to reconstruct the full solution of the binary system (there is no need of tie-line parameterization), refer *Fig. 4.1*.

As we move to a system with more than 2 components, the injection and the initial composition lie on different tie-line and the solution for the transport problem is constructed by tracing an appropriate non tie-line path ensuring conservation. The prolongation operator (A2F) for such multicomponent system is constructed based on the description given in section 3.3.2.



Figure 4.2: Shock reconstruction for a ternary system based on multi-scale technique in vaporizing gas drive (a) Light Component-CH4 (b) Heavy Component-C10



Figure 4.3: Shock reconstruction for a quaternary system based on multi-scale technique (a) Vaporising gas drive-CH4 (b) Condensing gas drive-CO2

Fig. 4.2 describes the reconstructed shock solution of a 3-component system (vaporizing gas drive) and Fig. 4.3 shows the reconstructed shock solution for a 4-component system (vaporising and condensing gas drive). The results of the reconstructed solution is evaluated by comparing it with a reference fine scale solution. We observed that the shock positions are accurately reconstructed at a fine scale accuracy with the use of A2F operator. On the other hand, the solution between the shocks (in the two phase region) is very different from the fine scale solution (Fig. 4.3). Though there is a valid reason behind this mismatch (discussed in appendix A.2), the same can be neglected since our objective is limited to the accuracy of shock solution.

On the basis of shock definition, it is can be understood that their position in space is invariant with respect to different components present in the system. In other words, the shock position of a global system can be identified by solving the conservation equation pertaining to a single component in that respective system. Based on this underlying principle, it is sufficient to perform the described reconstruction methodology of shocks on any single component of the entire system, thereby making the approach beneficial from performance point of view.

Reconstruction of Shock Solution - Multilevel

The multiscale based approach gives us a freedom to construct the solution at different grid resolutions by using the same prolongation operator, as they tend to remain invariant and changes only with change in the hydrodynamic parameters. Below, you can see an example of reconstructed the shock positions at different grid resolutions using the same A2F operator.



Figure 4.4: Shock reconstruction based on multi-scale technique, Vaporising gas drive (a) Heavy Component-C4 (b) Heavy Component-C10



Figure 4.5: Shock reconstruction based on multi-scale technique at different grid resolutions, Vaporising gas drive (a) Heavy Component-C4 (b) Heavy Component-C10

Fig. 4.5 shows a comparison of shock positions on different grid resolutions. The difference between the two solution curves are explained by the difference in their spatial resolution, higher resolution leads to more accurate results.

4.1.2. Reconstruction of Two-Phase Region

Once the shock positions are located in space, the solution lying in the region outside the shocks (single phase) are directly reconstructed using the AS operator developed based on a conservative coarse scale solution. This technique is relatively straightforward and in line with the framework proposed in [16]. Now the solution for the two-phase region is reconstructed by solving the modified conservation equation in the parameterized space, which has evolved as a result of the compositional space parameterization technique.



Figure 4.6: Reconstructed 2-phase region, Vaporising gas drive (a) Light Component-CH4 (b) Heavy Component-C10 (c) Heavy Component-C4 (d) Intermediate Component-CO2

Fig. 4.6 shows the solution of a vaporizing gas drive problem. It can be seen that the reconstructed two phase region (Z-CSP curve in Fig. 4.6) accurately matches with the reference fine scale solution. It is also worth noticing that the reconstructed solution of the entire n_c components are obtained by solving the coarse representation of the system ($\sigma \& v$) instead of $n_c - 1$ conservation equations. The decoupling between the thermodynamic and hydrodynamic problem provides an easier platform to carry out multi-dimensional analysis and sensitivity studies, since the γ -path is independent of flow properties and it is sufficient if we just solve the material balance equation to construct the full solution, skipping the Equations of state (EoS) computations.

Reconstruction of Two-Phase Region - Multilevel

Similar to the shock reconstruction at multilevel, the CSP technique is also implemented to reconstruct the solution of two phase region at different grid resolutions. *Fig. 4.7* shows the reconstructed solution of the transport problem on coarse scale and the same is compared with an reference coarse scale solution. The reconstructed coarse scale results are also plotted in tandem with the fine scale results (*Fig. 4.8*) for further study.



Figure 4.7: Reconstructed 2-phase region at Coarse Scale, Vaporising gas drive (a) Light Component-CH4 (b) Intermediate Component-CO2



Figure 4.8: Reconstructed 2-phase region at grid different resolutions, Vaporising gas drive (a) Light Component-CH4 (b) Intermediate Component-CO2

Based on the reconstructed results, we can observe that the two phase region is associated with a lot of intricacies with respect to compositional changes. Hence, it is preferable to carry the two phase reconstruction at a high spatial resolution. Under the CSP technique, this is quite affordable in terms of implementation, since the system involves coarser representation (2 equations).

Multiscale Reconstruction of System with Large Number of Components

This section describes an application of the developed reconstruction technique to a truly multicomponent system (5 components to be precise). The methodology described earlier remains valid irrespective of the size of the system, except for the fact that the dimensional space of the γ -path changes accordingly. The γ -path for a 5-component system is shown in *Fig. 4.9*.



Figure 4.9: Parameterized space (y-path) of 5C system, Vaporizing gas drive

We observe that, for a 4-component system, the γ -path exists in a 2D space (*Fig. 3.6*), whereas for a 5-component system, the γ -path exists in a 3D space (*Fig. 4.9*). 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 [10]. The nonlinear framework described earlier to solve for $\sigma \& v$, is used to construct the solution of this multicomponent system. The reconstructed simulation results are shown in *Fig. (4.10)* below.



Figure 4.10: Reconstructed 2-phase region of 5C system, Vaporising gas drive (a) Light Component-CH4 (b) Intermediate Component-CO2 (c) Heavy Component-C4 (d) Heavy Component-C6 (e) Heavy Component-C10

4.2. Reconstruction of Transport Problem - Upscaling

The upscaling framework, built on the basis of classical averaging techniques were also implemented to optimize the performance of compositional solvers. These techniques results in a coarse scale solution of the fine scale problem and constitute a single stage computational process. *Fig. 4.11* shows the upscaled solution of a condensing gas drive problem.



Figure 4.11: Reconstruction of full solution based on up-scaling technique, Condensing gas drive (a) Heavy Component-C4 (b) Intermediate Component-CO2 (c) Heavy Component-C10 (d) Light Component-CH4

Based on the plots it can be seen that the solution of the two phase region is reconstructed at an fine scale accuracy, while the solution near the shock regions is less accurate. This mismatch around the shock region can be explained by the fact that the shocks are generally characterized by a sudden jump in saturations/compositions, and in order to capture these sharp changes, the resolution in those regions needs to be comparatively high. But the upscaling technique leads to coarsening of the problem, thereby explaining the variance in the solution near the shock region.





Figure 4.12: Reconstruction of full solution based on up-scaling technique, Vaporising gas drive (a) Light Component-CH4 (b) Heavy Component-C10 (c) Heavy Component-C4 (d) Intermediate Component-C02

4.3. Discussion

In this research work, a systematic methodology to reconstruct the solution of a compositional transport problem is presented. On the basis of the results obtained by the means of two contrasting framework of implementation, it can be observed that the upscaling methodology is straightforward in terms of reconstructing the transport solution when compared with the multiscale technique. On the other hand, they are computationally inefficient and lack robustness in their approach.

The structure of the upscaling framework is such that they are strongly dependent on the results of global fine scale problem. To generate the reconstructed coarse scale results, we need the solution of (n_c-1) conservation equations on the fine scale. If one is satisfied with the accuracy of the upscaled results, they can be partially used in the multiscale reconstruction process.

On the other hand, the multiscale technique is an operator based approach where specially constructed operators are used to reconstruct the solution. They are robust in terms of application and invariant with respect to changes in the input hydrodynamic parameters of the system. The invariance is explained by the fact that the decoupling between the thermodynamics and the hydrodynamics of the compositional problem in the multiscale approach results in a constant γ -path [3]. Once the prolongation operators and the tie-line space have been constructed, the multiscale framework enables us to reconstruct the solution on multilevel resolutions with appropriate accuracy. Also, the adaptive usage of the multiscale operators on different solution regions and subsequent stage-wise reconstruction of the entire solution makes the multiscale technique more sensible and beneficial in terms of performance.

5

Future Work

The multiscale technique, proposed for improving the compositional simulation looks prospective and offers a great potential for practical applications. The primary advancement that can be made to the existing framework is to include complex nonlinear physics like compressibility and capillarity to the problem, and eventually develop a fully implicit (FIM) simulation framework.

Further, an Equation of State (EoS) model can be directly incorporated to determine the phase behavior and fluid properties of the system, thereby introducing the dependency of phase equilibrium relations on composition. It is important to note that, the CSP framework developed for acceleration of the phase behavior computations is independent of the type of EoS model.

Additionally, it should also be noted that the framework presented in this research work is developed for isothermal two phase system. Hence, there is also a possibility to generalize this ideology to a system consisting of arbitrary number of phases [1] & [8]. While the current implementation is limited by one-dimensional models, an extension to a more realistic 3D reservoir models is another important improvement. Likely, this extension seems quite straightforward since all CSP methodology was developed and tested for truly multi-dimensional reservoir models.

It would also be interesting to extend this framework on varied scientific applications, thereby examining the versatility of the technique. For instance, modeling and optimizing of thermal compositional problem can be captivating, though they pose significant challenges in the form of coupling between the mass balance, energy balance and phase behavior of the system.

6

Conclusion

A compositional simulator is a crucial tool to design oil recovery processes (especially to model the various enhanced oil recovery projects). The system is described on the basis of nonlinear conservation equations and associated constraints, thereby making them extremely large. Hence, the solution to this multiphase multicomponent problem is excessively time consuming and computationally inefficient. In this research work, we have developed and investigated a *multiscale* and *upscaled* based framework to solve the compositional problem in an efficient way.

The multiscale technique is based on the local saturation profile of the system and eventually a two stage reconstruction of the transport problem is carried out. The approach for predicting the shock positions in space on the basis of A2F operator is contemporary. As demonstrated, they are found to be effective and accurate on a wide range of gas injection problems, including the vaporizing and condensing gas drives. Subsequently, an advanced framework was developed to solve the compositional problem in the tie-line space (Compositional Space Parameterization) in order to reconstruct the solution in the two phase region. As a consequence of the parameterization, the n_c -1 conservation equations, that were formerly solved in each grid block, is reduced to 2 equations. It is worth noticing that the advanced framework used in solving the problem in tie-line space was built based on the ideas originated from the Method of Characteristics (MOC) based theory of gas injection process [13] & [27] and tie-line based parameterization technique proposed in [10] & [28].

On the other hand, the upscaled framework grounded over the classical averaging methodology involves simple and straight forward implementation. The drawback of this technique is its excessive dependency on global fine scale solution and eventually lacks of robustness. Hence, the multiscale technique is favored to meet the objective of reconstructing the solution of transport problem. The results, obtained based on both the multiscale and upscaled approaches, are compared against the fine scale solution of compositional problem. While the multiscale approach is found to be rewarding, there is also a lot of possibility for its further improvements for practical applications. The first and the foremost advancement would be to implement this technique on fully implicit framework involving complex nonlinear physics and multidimensions (3D reservoirs). The equations of state can also be directly incorporated, to model the phase behavior of the system. Further, it will be significantly useful and challenging to extend the proposed technique for systems with an arbitrary number of phases.



Appendix

A.1. Simulation Parameters

	2 Component System		
Composition	CH4	C10	
Initial Oil Composition	0.10	0.90	
Injection Gas Composition	0.999	1e-3	
K-Value	2.5	0.05	

Table A.1: Binary System, Vaporizing Gas Drive

	4 Component System			
Composition	CH4	CO2	C4	C10
Initial Oil Composition	0.10	0.18	0.37	0.37
Injection Gas Composition	0.997	1e-3	1e-3	1e-3
K-Value	2.5	1.5	0.5	0.05

Table A.2: Quaternary System, Vaporizing Gas Drive

	4 Component System			
Composition	CH4	CO2	C4	C10
Initial Oil Composition	1e-3	1e-3	0.491	0.507
Injection Gas Composition	0.624	0.374	1e-3	1e-3
K-Value	2.5	1.5	0.5	0.05

Table A.3: Quaternary System, Condensing Gas Drive

	5 Component System				
Composition	CH4	CO2	C4	C6	C10
Initial Oil Composition	0.10	0.18	0.20	0.17	0.35
Injection Gas Composition	0.996	1e-3	1e-3	1e-3	1e-3
K-Value	2.5	1.5	0.5	0.3	0.05

Table A.4: Multicomponent System (5C), Vaporizing Gas Drive

A.2. Analytical Fractional Flow - Non Tie-line Rarefaction

The construction of a fractional flow solution curve is similar to the construction of compositional path as described in section (2.4), where there is a series 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. A.1*) is constructed in compliance with the conservation laws as shown in *Fig. A.1*.



Figure A.1: Analytical fractional flow Curve, Solution based on non tie-line rarefaction

The cardinal difference between the traced solution curve that 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, on the other hand, it is extremely difficult to accurately locate the non tie-line points (pink dots) on these curves. The reconstruction of shock positions in space, which is the primary objective of this technique is highly sensitive to these points and even a marginal error in the construction of non tie-line path influences the accuracy of shock reconstruction in space.

It is for this reason 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 (: it is sufficient enough to accurately construct or trace the fractional flow solution curve with respect to the shock regions). Hence, the compositional changes within the two-phase region is sporadic in nature.

A.3. Solution Invariance - CSP

The modified conservation equation based on the CSP framework can be written in the dimensionless form as shown below,

$$\frac{\partial Z}{\partial t_D} + \frac{\partial F}{\partial x_D} = 0, \tag{A.1}$$

$$\frac{\partial \alpha(\gamma)Z + \beta(\gamma)}{\partial t_D} + \frac{\partial \alpha(\gamma)F + \beta(\gamma)}{\partial x_D} = 0$$
(A.2)

where, α is the slope and β are the intercept of the tie-line. The conservative nature of the modified equ. (A.1)-(A.2) allows the introduction of flowing potential, which is in turn defined by:

$$\overline{\phi(x_D, t_D)} = \int_{0.0}^{x_D, t_D} (Fdt_D - Zdx_D)$$
(A.3)

$$\overline{\psi} = x_D - t_D \tag{A.4}$$

where $\overline{\phi}$ is defined as the flowing volume of i-th component over an arbitrary volume and $\overline{\psi}$ is defined as the flowing volume of overall mixture. The composition and the fractional flow of the system is also represented in terms of these flowing potential as described in equ. (A.5).

$$Z = -\frac{\partial \overline{\phi}}{\partial x_D}, \qquad F = \frac{\partial \overline{\phi}}{\partial t_D}$$
(A.5)

Based on these potential definitions, the function β follow the conservation law [3] of the form:

$$\int_{\partial\Omega} (\alpha_i d\overline{\phi} - \beta_i d\overline{\psi}) = 0 \tag{A.6}$$

On the other hand, the integral form of the modified conservation equ. (A.1)-(A.2) is defined as shown in equ. (A.7).

$$\int_{\partial\Omega} (\alpha_i F + \beta_i) dt_D - (\alpha_i Z + \beta_i) dx_D = 0$$
(A.7)

On expanding the integral and rewriting the equation (A.7) in terms of the potential functions, we get:

$$\int_{\partial\Omega} \alpha_i (Fdt_D - Zdx_D) - \beta_i (dx_D - dt_D) = 0$$
(A.8)

which, further reduces to the form:

$$\int_{\partial\Omega} (\alpha_i d\overline{\phi} - \beta_i d\overline{\psi}) = 0 \tag{A.9}$$

It can be observed that the equ. (A.9), representing the integral form of mass conservation equation, is exactly similar to the conservation form of the tie-line parameters (equ. A.6). Now, based on the integral conservation law, the equation (A.9) follows the system of partial differential equation of the form:

$$\frac{\partial A_i(\gamma)}{\partial \overline{\phi}} + \frac{\partial B_i(\gamma)}{\partial \overline{\psi}} = 0, \tag{A.10}$$

and the same is referred to as the auxiliary equation or the thermodynamic problem of a compositional system, and it is decoupled with the hydrodynamics of the system.

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