ADVANCED DISCRETIZATION FRAMEWORK FOR
FULLY-IMPlicit SIMULATION OF MULTIPhysics FLOW IN POROUS MEDIA

by
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FULLY-IMPLICIT SIMULATION OF MULTIPHYSICS FLOW IN POROUS MEDIA

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A DISSERTATION
APPROVED FOR THE DISCIPLINE OF
PETROLEUM ENGINEERING

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ABSTRACT

Jiamin Jiang (Doctor of Philosophy in Petroleum Engineering)
Advanced Discretization Framework for Fully-Implicit Simulation of Multiphysics Flow in Porous Media
Directed by Rami Younis
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(542 words)

This work covers several advances in numerical discretization methods for reservoir simulation. In the presence of counter-current flow, nonlinear convergence problems may arise in implicit time-stepping when the popular Phase-Potential Upwinding (PPU) scheme is used. The PPU numerical flux is non-differentiable across the co-current/counter-current flow regimes. This may lead to cycles or divergence in the Newton iterations. Recently proposed methods address improved smoothness of the numerical flux. The objective is to devise and analyze an alternative numerical flux scheme called C1-PPU that, in addition to improving smoothness with respect to saturations and phase potentials, also improves the level of scalar nonlinearity and accuracy. C1-PPU involves a novel use of the flux limiter concept from the context of high-resolution methods, and allows a smooth variation between the co-current/counter-current flow regimes. The scheme is general and applies to fully coupled flow and transport formulations with an arbitrary number of phases. We analyze the consistency property of the C1-PPU scheme, and derive saturation and pressure estimates, which are used to prove the solution existence. The numerical examples show that the C1-PPU scheme exhibits superior convergence properties for large time steps compared to the other alternatives.
The first-order methods commonly employed in reservoir simulation for computing the convective fluxes introduce excessive numerical diffusion leading to severe smoothing of displacement fronts. We present a fully-implicit Cell-Centered Finite-Volume (CCFV) framework that can achieve second-order spatial accuracy on smooth solutions, while at the same time maintaining robustness and nonlinear convergence performance. A novel multislope MUSCL method is proposed to construct the required values at edge centroids in a straightforward and effective way by taking advantage of the triangular mesh geometry. In contrast to the monoslope methods in which a unique limited gradient is used, the multislope concept constructs specific scalar slopes for the interpolations on each edge of a given element. Through the edge centroids, the numerical diffusion caused by mesh skewness is reduced, and optimal second order accuracy can be achieved. Moreover, an improved smooth flux-limiter is introduced to ensure monotonicity on non-uniform meshes. The flux-limiter provides high accuracy without degrading nonlinear convergence performance.

Although many works confirm the high accuracy of Embedded Discrete Fracture Model (EDFM) for the solutions of pressure and velocity field, very few results have been presented to examine its accuracy for the saturation solutions from multiphase flow problems. Our study shows that EDFM can induce large errors for multiphase displacement processes, due to its incapability to capture the proper flux split through a fracture. For the first time in the literature we present a systematic evaluation on the performances of EDFM for multiphase flow and provide a detailed analysis to illuminate when and why the method fails. The analysis motivates us to exploit the projection-based extension of EDFM (pEDFM) as an effective method to resolve the limitations associated with EDFM. Moreover, we make several improvements upon the original pEDFM method. A physical constraint on the preprocessing stage is proposed to overcome the limitation in a naive implementation of pEDFM. A number of test cases with different fracture geometries are presented to benchmark the performances of the improved pEDFM method for multiphase flow. Grid convergence studies are conducted for different numerical schemes. The results show that improved pEDFM significantly outperforms the original EDFM method.
ACKNOWLEDGEMENTS

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I would like show my greatest appreciation to family for their unconditional support and love. This work is dedicated to my wife and my parents.
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CHAPTER 1
INTRODUCTION

1.1 Background

Numerical reservoir simulation is an important tool that facilitates improved management and design of applications such as oil and gas recovery, groundwater remediation, and CO$_2$ subsurface sequestration. Predicting the evolution of the fluid phase pressure and saturation fields involves solving the partial differential equations (PDEs) governing multiphase flow and transport in porous media. Solving these PDEs for high-resolution reservoir models describing realistic geology is challenging. The evolution of the transport problem are highly nonlinear. Specifically, the transport equations in the presence of viscous and buoyancy forces are characterized by non-convex and non-monotonic flux functions (Li and Tchelepi 2015). These features make the design of robust, efficient and accurate numerical discretization schemes challenging.

Several temporal discretization methods are available to solve the conservation equations (Aziz and Settari 1979). The use of explicit temporal scheme poses severe restrictions on the timestep size, and is usually considered impractical due to the large variations of magnitude in the velocity field and the cell pore volumes (porosity) throughout the domain. Implicit schemes such as the Fully Implicit Method (FIM), or the Sequential Implicit Method (SIM), are attractive in these situations. A Newton-based strategy is commonly applied to solve the resulting nonlinear algebraic systems at each time step. Owing to this, nonlinear convergence problems may arise in implicit time-stepping. This is a major concern because of the severe negative impact on computational performance. When convergence failures are encountered, heuristic techniques are often employed to adaptively control the timestep, and upon failure to converge, the iteration is restarted with a smaller timestep, and the previous
computations are wasted (Younis et al. 2010).

Often, reservoir simulation schemes use single-point upstream weighting for the computation of the convective fluxes when multiphase fluids are present. These schemes are only first-order accurate and may cause high viscosity effects. Second-order schemes provide a better resolution and reduce the smoothing near shocks. The Monotone Upstream Scheme for Conservation Law (MUSCL) method was introduced by Van Leer (Van Leer 1979) to solve hyperbolic partial differential equations using the finite volume (FV) method. The main idea is to apply a piecewise linear reconstruction of the solution variables to achieve more accurate schemes that still preserve the stability property; e.g. the maximum principle or the Total Variation Diminishing (TVD) properties. Slopes are limited to prevent unphysical oscillations and various limiters in the 1-D context have been developed to obtain high-resolution TVD schemes (Buffard and Clain 2010).

However, even for a simple first-order method, solving a large nonlinear system is often very expensive; extra couplings and nonlinearity of the discretized equations can be introduced from a higher-order spatial discretization (Natvig and Lie 2008). It has been shown that strong nonlinearity as well as the lack of continuous differentiability in numerical flux function and flux limiter can cause serious nonlinear convergence problems (Li and Tchelepi 2015; Zhang et al. 2015).

Simulation of complex subsurface processes entails solution of multiphase flow, multicomponent transport of mass and heat. In addition, reactions and mechanical interactions with the solid have received significant attention. Having a reservoir simulation framework that is easily extensible to account for the additional physical interactions and ‘new’ transport mechanisms associated with Enhanced Oil Recovery (EOR) processes is quite important. To meet this objective, one has to address the important challenge of balancing the complexity of the flow physics with computational efficiency. Specifically, it is important to deal with the coupling across the different physical mechanisms while developing specialized discretization for the sub-problems.

One application target of a multiphysics platform is on naturally fractured reservoirs.
Petroleum reservoirs and aquifers are often highly heterogeneous and generally include preferential flow paths in the form of natural fracture networks (Mustapha 2014). The detailed understanding of multiphase fluid flow in such systems is of interest in many geoscience applications (Karimi-Fard and Durlofsky 2016). The high contrasts in the permeability and length-scale between matrix and fracture make it very challenging to modeling of flow behaviors in naturally fractured reservoirs (NFRs). This has led to increasing effort being devoted to the development of accurate and efficient numerical solution techniques.

Due to the rapid depletion in conventional resources of natural gas, unconventional reserves such as shale gas reservoirs have become more and more important for the energy industry in North American and have gradually turned into a major supplier of world energy demand in recent years. Shale gas production can be economically viable if sufficient stimulation of ultra-tight formation is achieved through the technologies of horizontal drilling and hydraulic fracturing. In order to obtain optimal management plans for shale gas reservoirs, there is considerable interest in numerical modeling approaches which can adequately characterize the complicated production behaviors, featured by multiscale single-phase (gas) and/or multiphase fluid (gas, gas condensate and/or brine) flow and transport in ultra-low permeability, highly heterogeneous porous/fractured, and stress-sensitive rocks (Wu et al. 2014). Compared with conventional reservoirs, fluid flows in unconventional reservoirs with ultra-low permeability involve non-linear adsorption/desorption, non-Darcy flow in the entire range from high flow rate to low flow rate, strong rock-fluid interaction, and rock/organic matter deformation within nanopores or micro-fractures.

1.2 Overview

The first part of this thesis covers several advances in the numerical discretization methods for reservoir simulation. Chapter 2 presents C1-continuous phase-potential upwind (C1-PPU) schemes for efficient simulation of fully-coupled multiphase flow with gravity. The novel schemes have several favorable properties compared to the other alternatives. Chapter 3 presents a fully-implicit high-resolution CCFV framework that maintains robustness and
nonlinear convergence performance. A novel multislope MUSCL method and an adaptive flux limiter is developed within the framework. In Chapter 4, an improved projection-based embedded discrete fracture model (pEDFM) is proposed. It has been shown that the novel method significantly outperforms the original EDFM method.

The second part of the thesis covers the multiphysics modelings with application to unconventional resource recovery. The objective is to exploit the existing discretization techniques for building a flexible platform to increase the robustness and expand the capabilities in handling complex physics. Chapter 5 presents a fully-coupled fluid flow and geomechanics model to accurately characterize the complex production behaviors of fractured shale gas reservoirs. The flow equations are discretized using a mimetic finite difference method, and poro-elasticity equations by a Galerkin finite-element approximation. In Chapter 6, a multicomponent compositional model is developed for gas-condensate shale reservoirs. Related mechanisms such as multicomponent apparent permeability (MAP), sorption and molecular diffusion are incorporated.

1.2.1 C1-continuous Phase-Potential Upwind (C1-PPU) Schemes

Given the possibility of divergence of Newton-like methods for general problems, a number of heuristic strategies have been devised to safeguard the Newton updates. A common idea across these methods is to apply a cell-by-cell damping factor to limit large changes in the Newton updates. For example in the commercial simulator Eclipse (Schlumberger 2008), no saturation change in a cell that is greater than some small amount in magnitude is allowed; the tolerance is usually chosen to be 0.2. Jenny et al. (2009) developed a physics-specific nonlinear solver for the two-phase viscous-dominant flow. They used the inflection point of the analytical flux (fractional-flow) function to guide the Newton-based iterative updating of the saturation field. Wang and Tchelepi (2013) extended the strategy to flows that include both viscous and buoyancy forces. They introduced trust region analysis based on the analytical flux function to guide the Newton iterations. However, as argued by Li and Tchelepi (2015), the trust regions should be those of the numerical flux function, because the
analytical form does not fully reflect the complex nonlinear behavior of a discretized system, especially when counter-current flow exists due to buoyancy and capillarity.

In parallel to the efforts on ad hoc safeguarding strategies, the influence of the spatial discretization technique on the solubility of the residual system is a topic of interest. Phase-Potential Upwinding (PPU) schemes are widely used in reservoir simulation practice. In PPU schemes, the upstream direction of a fluid phase is determined according to the gradient of its potential across the interface between two computational cells. Recent studies show that in the presence of counter-current flow due to buoyancy, nonlinear convergence problems may be pronounced when the popular PPU scheme is used to approximate the numerical flux (Li and Tchelepi 2015; Lee et al. 2015; Lee and Efendiev 2016). The PPU numerical flux is non-differentiable across the co-current/counter-current flow regimes and may thus lead to oscillations or even divergence in the Newton iterations. Lee et al. (2015) proposed a continuously differentiable numerical flux scheme called Hybrid Upwinding (HU) to address the discontinuous behavior due to flow reversal.

In the design of numerical flux calculations for transport problems, both the level of nonlinearity and the C1-continuity can have dramatic effects on the nonlinear convergence of the solution for the timestep. The objective of this topic is to devise and analyze an alternative numerical flux scheme called C1-PPU that allows a smooth variation between the co-current/counter-current flow regimes as well as an optimal balance between the scalar nonlinearity and accuracy of the flux function. C1-PPU involves a novel use of the flux limiter concept from the context of high-resolution methods. The consistency and monotonicity properties of the C1-PPU flux for two phase transport problem are examined. We also propose a generalization of C1-PPU to coupled flow and transport with an arbitrary number of phases. We derive saturation and pressure estimates, and prove the existence of a solution. We show that the generalized C1-PPU scheme is continuously differentiable with respect to saturations as well as phase potentials, and it can efficiently handle the coupled formulation of mass conservation equations.

Numerical examples including 1D scalar transport and 2D heterogeneous problems
with fully-coupled multiphase flow and transport are presented. The results indicate that in addition to smoothness, scalar nonlinearity may also be critical for convergence behavior and thus needs to be considered in the design of an efficient numerical flux scheme. Moreover, the results show that the C1-PPU scheme exhibits superior convergence properties for large time steps compared to the other alternatives.

### 1.2.2 Multislope MUSCL Method

While in principle, MUSCL schemes are applicable to unstructured meshes, not all of the required data is readily available on the meshes, and the solution may suffer from large numerical diffusion due to mesh skewness (Denner and van Wachem 2015). Several high-resolution formulations were presented in the literature to solve the multiphase transport problem in porous media (Durlofsky 1993; Edwards 2006; Natvig and Lie 2008; Lamine and Edwards 2008; Geiger et al. 2009; Schmid et al. 2013).

Cell-Centered Finite-Volume (CCFV) discretizations may offer several attractive features, especially for fluid flow in heterogeneous or fractured porous media (Edwards 2006; Monteagudo and Firoozabadi 2007; Hoteit and Firoozabadi 2008; Geiger et al. 2009). The objectives of this work are to develop a fully-implicit CCFV framework based on a novel multislope MUSCL method and an adaptive limiting strategy that have improved computational efficiency, smoothness properties, and accuracy. In contrast to the classical monoslope method in which a unique limited gradient is used within a given element, the multislope method carries out the limiting process by dealing with 1-D situations for each edge (Hou et al. 2014). The reconstruction scheme interpolates the required values at the edge centroids in a simple way by taking advantage of some geometric features of the triangular mesh. Through the edge centroids, the numerical diffusion caused by mesh skewness is reduced, and optimal second-order accuracy can be achieved. An improved gradually-switching piecewise-linear flux-limiter is introduced according to mesh non-uniformity in order to prevent spurious oscillations. The smooth flux-limiter provides high accuracy without degrading nonlinear convergence performance.
For the discretization of pressure and Darcy velocities, a Mimetic Finite Difference (MFD) method that provides flux-continuity and an accurate total velocity field is used. The fully-coupled MFD-MUSCL framework is adapted to accommodate a lower-dimensional Discrete Fracture-Matrix (DFM) model. Several numerical tests with discrete fractured systems are carried out to demonstrate the efficiency and robustness of the numerical model. The results show that the high-order schemes effectively reduce numerical diffusion, leading to improved resolution of saturation fronts compared with the first-order scheme. In addition, it is demonstrated that the proposed multislope method and adaptive flux limiter exhibit superior nonlinear convergence compared with other alternatives.

1.2.3 Improved Projection-based Embedded Discrete Fracture Model

Broadly, two classes of numerical approaches are commonly used in the literature to perform flow simulations for NFRs: 1) Continuous representations in the form of variants of a dual-porosity/dual-permeability (DP/DK) approach, and 2) Discrete representations in the form of discrete fracture-matrix (DFM) method.

DP/DK models (Warren and Root 1963; Kazemi et al. 1976) have traditionally been used for the last few decades, but there are some fundamental assumptions underlying the models which greatly restrict their applicability to represent real fracture networks (Geiger et al. 2009). Continuum types of models are applicable if the fracture system is connected extensively. Also the applications typically assume that the properties and geometry of the fracture network remain relatively constant (Norbeck et al. 2016). DP/DK models tend to homogenize the fractures contributing to flow in each simulation block by ignoring their connectivity; thus unphysical fracture flows could be established between disconnected areas of the reservoir (Panfili et al. 2015). Moinfar et al. (2011) demonstrated examples where the DK model fails to provide satisfactory solutions in the presence of fracture system with high heterogeneity. Another shortcoming is that DP/DK models treat matrix and fracture as two parallel continuous systems coupled by transfer functions. These transfer terms depend on the shape factor, which is not straightforward to be determined for the problems involving
capillarity, gravity and the multi-component and -phase systems (Geiger et al. 2013).

In recent years, the discrete fracture-matrix (DFM) approach has grown in popularity as a more accurate alternative for the modeling of NFRs. To overcome the deficiencies of continuum models, DFMs attempt to explicitly incorporate fractures as discrete representations. Subsequently, they can be used to simulate realistic and complex fracture geometries, and to accurately account for the effects of individual fractures on fluid flow (Jiang and Younis 2016). Moreover, the specification of the exchange between matrix and fracture is relatively straightforward since it depends directly on the fracture geometry (Jiang and Younis 2017). A large variety of DFMs is available in the literature (for example, Kim and Deo 2000; Juanes et al. 2002; Karimi-Fard and Firoozabadi 2003; Karimi-Fard et al. 2004, 2006; Monteagudo and Firoozabadi 2004; Reichenberger et al. 2006; Hoteit and Firoozabadi 2006, 2008; Eikemo et al. 2009; Matthei et al. 2007, 2010; Geiger et al. 2009; Sandve et al. 2012; Schmid et al. 2013; Maier and Geiger 2013; Fumagalli and Scotti 2013, 2014). Most DFM models rely on unstructured grids to conform to the geometry of fracture networks (Moinfar et al. 2013). However, the application of conforming grids at field scale is limited due to the associated prohibitive computational cost. The grid generated for an arbitrary fracture network is usually composed of many elements with small size and poor quality, which could badly affect the numerical solutions (Mallison et al. 2010; Mustapha 2014).

In addition to the classical models, Lee et al. (2001), Li and Lee (2008), Hajibeygi et al. (2011) and Moinfar et al. (2013, 2014) introduced and extended an embedded discrete fracture model (EDFM) that incorporates the effect of each fracture explicitly without requiring the simulation grid to conform to the fracture geometry. EDFM could achieve a compromise between accuracy and efficiency by enabling the use of standard corner-point grids for the background matrix, together with a discrete representation of the fracture segments that intersect matrix cells (Fumagalli et al. 2016). EDFM borrows the concept of transport index to tie the additional computational control-volumes for fractures to matrix. Recent works on the implementations of EDFM for different types of problems include Panfili et al. (2015), Jiang and Younis (2016), Tene et al. (2016), Norbeck et al. (2016) and
Fumagalli et al. (2016, 2017). It should be noted that EDFM is not suitable in cases when fracture permeability lies below that of matrix, as recently revealed by Tene et al. (2016). To resolve this limitation, they propose a projection-based extension of EDFM (pEDFM), which can accommodate to discrete features with a wide range of permeabilities (i.e. from highly conductive fractures to flow barriers).

Although many numerical experiments have confirmed that EDFM is accurate for the solutions of pressure and velocity field, very few results have been presented to investigate its accuracy for the saturation (or component) solutions obtained from multiphase flow problems. In the result sections we will show that with the current implementation of EDFM, large errors can be induced for multiphase displacement processes, due to the unphysical fluxes inherent in the method. For the first time in the literature we present a systematic evaluation on the performances of EDFM for multiphase flow and provide a detailed analysis to illuminate when and why the method fails. Based on the observation that EDFM is unable to separately capture the fluxes on the two sides of a fracture, the recently proposed pEDFM method is examined and exploited. Through some preliminary testings we find that pEDFM can be an effective method to resolve the limitations of EDFM. It is worth to point out that the projection concept in pEDFM is originally introduced to address the issue of flow barrier, and only the results for single-phase flow are given in the work of Tene et al. (2016). Moreover, we make several improvements upon the original pEDFM method. One important aspect is that unphysical solutions may arise with a naive implementation of pEDFM and thus we propose imposing a constraint on the preprocessing stage for creating the extended fracture-matrix fluxes.

We present a number of test cases that contain different fracture geometries to benchmark the performances of the improved pEDFM method for multiphase flow. Grid convergence studies are also conducted for different methods. The results demonstrate that improved pEDFM significantly outperforms the original EDFM method. Compared to the first-order convergence rate of improved pEDFM, EDFM exhibits terrible convergence with zeroth-order. Moreover, improved pEDFM has a similar performance with the unstructured
1.2.4 Coupled Flow and Geomechanics Modeling

Compared with conventional reservoirs, gas flow in shale formation is affected by additional nonlinear coupled processes including gas adsorption, low-permeability non-Darcy flow and matrix/fracture deformations (Jiang and Younis 2015; 2016; Ren et al. 2017).

Darcy’s law, which describes viscous flow driven by pressure gradient, is applicable to porous media where continuum theory holds and fluid velocity could be approximated as zero at the pore wall (Javadpour et al. 2007). However, the fluid-continuum theory is no longer valid for shale reservoirs with pore radius in the range of nanometers (Florence et al. 2007). Dynamic apparent permeability models are extensively employed to reflect the flow regimes associated with the non-Darcy effect (Wu et al. 2014). The adsorbed gas layer on the pore surface occupies the pore space, resulting in the variations of the gas apparent permeability (Xiong et al. 2012; Cao et al. 2016).

In addition, stress-sensitivity is another active phenomenon in shale gas reservoirs. During reservoir depressurization, the pore pressure decline leads to a rise in the effective stress which, subsequently compacts pore-structure geometry and reduces formation porosity and intrinsic permeability (Ren et al. 2016). In the meantime, gas desorption triggers matrix shrinkage, whose effect is contrary to the pore pressure decrease (Cui and Bustin 2005; Zhang et al. 2008). Consequently, the net change in porosity and permeability accompanying gas extraction is controlled by the several competing processes (Cao et al. 2016). The nonlinear and stress-sensitive flow phenomena can be further aggravated by the generation of complex fracture network with non-ideal geometries after the fracturing treatment. It has been reported that the sharp decline of the gas rate within the first few months of production is one of the distinguishable features exhibited by the fractured stimulated wells (Fan et al. 2015). The stimulation process involves injecting high-pressure fracturing fluid, together with proppants which are usually sand or ceramic particles, into shale reservoir to break down the rock. Proppants play the role of keeping the fracture open after pumping
stops and fracturing fluid flows back to the surface (Han et al. 2016). The proppant layers filling the fracture channels can create highly conductive flow paths for gas production (Chen et al. 2017). Under the effects of pressure decline and high confining stresses on the fracture faces, proppant compaction, embedment into shale rock, and even crushing may occur, causing fracture closure and thus substantial production loss. Several studies have proposed the purely elastic models for the contacts between proppant and fracture (Khanna et al. 2012; Li et al. 2015; Li et al. 2016; Chen et al. 2017). Hertzian theory (Hertz 1882) is widely applied for purely elastic contacts, but in most cases there are plastically deforming behaviors which extremely complicate the contact force-displacement relationship (Ghaednia et al. 2016). Under high compressive stress, proppant failure (crushing) can be initiated. Hertzian theory does not work properly when the vertical displacement is large relative to the radius of proppant sphere. Therefore in this work we develop a comprehensive proppant-fracture model which is based on the theories of elasto-plastic contact mechanics, to accurately capture the proppant embedment and crushing phenomena.

A fully coupled fluid flow and geomechanics model is developed to simulate the stress field and gas production in fractured shale reservoirs. A unified model for gas flow in organic nanopores is implemented, accounting for the coupling mechanisms of the non-Darcy flow regimes, adsorption layer and stress dependence. The flow equations are discretized using a mimetic finite difference method, and the poro-elasticity equations by a Galerkin finite-element approximation. The discrete fracture-matrix (DFM) model based on a conformal unstructured grid is employed to represent a fracture as the interface between two neighboring cells. The nonlinear contact problem between the two fracture planes is introduced to describe the fracture mechanics behavior. A splitting nodes technique is used such that each node along the fracture interface is assigned to double nodes with the same coordinates, for overcoming the explicit discontinuities in the fractured domain (Garipov et al. 2016).

The developed multiphysics simulator allows us to examine which factors have the most significant impact on the gas recovery of shale formations. High fidelity numerical solutions are provided to characterize the rate-transient signatures in the presence of the
different flow and geomechanical mechanisms.

1.2.5 Compositional Modeling of Fractured Shale Gas-Condensate Reservoirs

Due to recent low gas prices, most of the operating companies have slowed down their activities in dry gas areas and refocused their attention on production from the gas-condensate window of liquid-rich regions (Fathi et al. 2013). The Eagle Ford, Barnett and Woodford shale in the U.S., and the Duvernay Shale in Canada are examples of liquid-rich shale (LRS) plays which are being exploited to produce more profitable liquid hydrocarbons with natural gas. However, this change in production plans requires detailed investigation of gas condensate bank development and saturation dynamics in the formation. An advanced level of understanding of the parameters and mechanisms affecting condensate recovery is necessary for achieving optimal development and operation plans. As the pressure in near-wellbore region drops below the dew-point, liquid droplets are formed and tend to be trapped in small pores; thus condensate blockage would occur and lead to a rapid decline in well productivity. It has been suggested that injection of CO2 into shale gas reservoirs can be a feasible option to enhance recovery of natural gas and/or valuable condensate oil, while at the same time sequestering CO2 underground (Godec et al. 2013; Eshkalak et al. 2014; Ren et al. 2015). Two methods are usually employed in the context of gas injection: gas flooding and huff-n-puff. Previous simulation studies showed that traditional well-to-well flooding for shale reservoirs might not be feasible because it is very difficult for the injected fluid to efficiently transport into the ultra-tight formation (Sanchez-Rivera et al. 2015). Therefore, it is advantageous to consider a cyclic huff-n-puff approach in which the same well alternates between injection and production. The injected CO2 is expected to serve two purposes: 1) miscible interaction with the condensate phase to reduce the dew point pressure and to improve oil mobility of the fluid system, and 2) repressurization of the reservoir so that pressure is raised above the dew point in near-wellbore region (Sheng 2015).

In order to achieve optimal development and operation plans for various enhanced oil
recovery scenarios in shale gas reservoirs, there is considerable and timely interest in numerical simulation techniques which can accurately predict the complex production phenomenon. Unfortunately, existing simulation techniques fail to include the evolving understanding of the recovery physics associated with the fluid system that consists of multiple gas species or phases. Transport properties and mechanisms as well as phase behavior under nanoscale confinement exhibit deviations from their bulk behavior. Multiflow mechanisms such as slip flow, transition flow and Knudsen diffusion may co-exist, thus apparent permeability should be used to correct the flow deviation from the traditional Darcy’s law (Li et al. 2015). Desorption has also been suggested to be an important storage mechanism in organic-rich shales, particularly for heavy hydrocarbon fractions, which may contribute significantly to condensate production (Haghshenas et al. 2014). Moreover, molecular diffusion may take over as the main recovery mechanism under the severe effect of condensate bank impairment in fractured gas-condensate systems (Ayala et al. 2006).

Many studies indicate that the thermodynamic phase behavior of in-situ hydrocarbon mixtures in confined spaces significantly deviates from that of bulk fluids in the PVT cells (Wang et al. 2013; Jin et al. 2013; Alharthy et al. 2013; Teklu et al. 2014; Wang et al. 2014; Jin and Firoozabadi 2015; Rezaveisi et al. 2015; Xiong et al. 2015; Tan and Piri 2015). The nanopores in the ultra-tight shale formation could lead to significant interfacial curvature and capillary pressure between confined vapor and liquid phases. The work of Nojabaei et al. (2013) shows that without considering the effect of capillary pressure in vapor-liquid equilibrium (VLE) calculation a conventional reservoir simulator will likely not be able to explain the inconsistent produced gas-oil ratio (GOR) observed in the field compared to simulated results.

In this work, we develop a comprehensive compositional simulator for the modeling of gas-condensate shale reservoirs with complex fractured system. Related storage and transport mechanisms such as multicomponent apparent permeability (MAP), sorption and molecular diffusion are considered. Extended Langmuir model is implemented to simulate the multicomponent sorption behavior, and the ordinary diffusion flux driven by concen-
tration gradient is considered in the form of Fick’s law. In order to accurately capture the complicated phase behavior of the multiphase fluids, an Equation of State (EOS) based phase package is incorporated into the simulator. The phase package takes into account the effect of the large capillary pressure that exists in ultra-tight shale matrix. A modified negative-flash algorithm that combines Newton’s method and successive substitution iteration (SSI) is used for phase stability analysis.

The developed simulator is used to understand and quantify the combined effect of capillary pressure and multicomponent mechanisms on the phase and production behavior in gas-condensate shale reservoirs. We present preliminary simulation studies to show the applicability of CO2 huff-n-puff for the purpose of enhanced hydrocarbons recovery. Several design components such as the number of cycles and the length of injection period in the huff-and-puff process are also briefly investigated.
CHAPTER 2
C1-CONTINUOUS PHASE-POTENTIAL UPWIND SCHEMES

2.1 Immiscible multiphase flow and transport in porous media

We consider compressible and immiscible flow and transport with $n_p$ fluid phases. The mass conservation equation for phase $\alpha$ is

$$\frac{\partial}{\partial t} (\phi \rho \alpha S \alpha) + \nabla \cdot (\rho \alpha u \alpha) = \rho \alpha q^W \alpha. \quad (2.1)$$

where $\alpha \in \{1, \ldots, n_p\}$. $\phi$ is the rock porosity. $\rho \alpha$ and $u \alpha$ are the density and velocity of each phase, respectively. $q^W \alpha$ is the well flow rate (source and sink terms). $S \alpha$ is phase saturation, with the constraint that the sum of saturations is equal to one

$$\sum_{\alpha} S \alpha = 1. \quad (2.2)$$

The phase velocities can be expressed using the multiphase extension of Darcy’s law

$$u \alpha = -k \lambda \alpha (\nabla p + \rho \alpha g \nabla h). \quad (2.3)$$

where capillary forces are neglected. $k$ is the scalar rock permeability. $p$ is pressure. $g$ is gravitational acceleration and $h$ is height. The phase mobility $\lambda \alpha (S_1, \ldots, S_{n_p}) = k_{ra} (S_1, \ldots, S_{n_p}) / \mu \alpha$. $k_{ra}$ and $\mu \alpha$ are the relative permeability and viscosity, respectively.

2.2 Fully-implicit finite-volume discretization

The coupled multiphase problem in Eq. (2.1) is highly nonlinear, and it can be chal-
lenging to solve the system for heterogeneous porous media. The method of choice for the
time discretization is often a backward, first-order Euler scheme. A standard finite-volume
scheme (Eymard et al. 2000) is employed as the spatial discretization for the mass conserva-
tion equations. Let \( \Omega \subset \mathbb{R}^{n_d} \) be the reservoir domain in dimension \( n_d \). The simulation
grid represents a partition of \( \Omega \) into a set of non-overlapping control volumes. A two-point
flux approximation (TFPA) is used to approximate the flux at a cell interface. It is assumed
that pressure varies linearly within each of the two adjacent cells. Let \( j \) denotes the set of
indices such that control volumes \( \Omega_i \) share an interface \( \Gamma_{ij} \) with control volume \( \Omega_j \). The
fully-implicit discretization of a cell can be written as

\[
R_A + R_F = R_W, \tag{2.4}
\]

where the accumulation, flux and well parts are

\[
R_A = \frac{|\Omega_i|}{\Delta t} \left( (\phi_i \rho_{\alpha,i} S_{\alpha,i})^{n+1} - (\phi_i \rho_{\alpha,i} S_{\alpha,i})^n \right), \tag{2.5}
\]

\[
R_F = \sum_{j \in \text{adj}(i)} \rho_{\alpha,ij}^{n+1} F_{\alpha,ij}^{n+1} (\Delta p_{ij}, S_i, S_j), \tag{2.6}
\]

\[
R_W = \rho_{\alpha,i}^{n+1} Q_{\alpha,i}^{W,n+1} (p_i, S_i). \tag{2.7}
\]

where \( i \in \{1, \ldots, N\} \) and the shorthand notation \( S_i = \{S_{k,i}\}_{k \in \{1, \ldots, n_p\}} \) refers to the saturations
in cell \( i \). \( \Delta t \) is the time step size. \( |\Omega_i| \) is the volume of cell \( i \). \text{adj}(i) denotes the set of indices
such that cell \( i \) share an interface \( \Gamma_{ij} \) with cell \( j \). \( \Delta p_{ij} = p_i - p_j \) is the pressure difference
between \( i \) and \( j \). The primary saturations are chosen to be the water saturation (respectively,
water and gas saturations) for two-phase (respectively, three-phase) flow, which is common
practice in reservoir simulation (Kwok and Tchelepi 2008). The discrete phase flux across
the interface is approximated by

\[ F_{\alpha,ij} = T_{ij} \lambda_{\alpha,ij} \left( \Delta p_{ij} + \bar{\rho}_\alpha g \Delta h_{ij} \right). \quad (2.8) \]

where \( \bar{\rho}_\alpha \) is the arithmetic average for the phase densities of the two cells. The phase mobility \( \lambda_{\alpha,ij} \) in the numerical flux is evaluated using first-order the upstream weighting schemes. The total face transmissibility \( T_{ij} \) that combines the two half-transmissibilities in a harmonic average is

\[ T_{ij} = \frac{T_i T_j}{T_i + T_j}. \quad (2.9) \]

The two-point half-transmissibility for a general grid is obtained by imposing flux and pressure continuity at the center of the interface.

Time discretization is carried out using a backward, first-order Euler scheme. At each time-step of an implicit simulation, given the current state, \( U^n \), and a fixed time-step size, \( \Delta t > 0 \), we seek to obtain the new state, \( U^{n+1} \), by solving the corresponding nonlinear residual system \( R \) using a standard Newton-Raphson method

\[ R \left( U^{n+1}; \Delta t, U^n \right) = 0. \quad (2.10) \]

Newton's method generates a sequence of iterates, \( [U^{n+1}]^\nu \), \( \nu = 0, 1, \ldots \), that hopefully converges to the new state, \( U^{n+1} \). Denoting the Jacobian matrix of the residual with respect to the new state as \( J \), this sequence is generated starting from the old state

\[ [U^{n+1}]^0 = U^n, \]

\[ [U^{n+1}]^{\nu+1} = [U^{n+1}]^\nu - J^{-1} R \left( [U^{n+1}]^\nu; \Delta t, U^n \right). \quad (2.11) \]

### 2.3 Upwinding schemes for immiscible two phase transport

In this section, the general multiphase system is reduced to an immiscible two-phase case (oil and water), for allowing a clearer analysis on the basic properties of different upwinding schemes. If we neglect the compressibility, the total velocity becomes fixed in 1D,
and the reduced problem can be written as a scalar hyperbolic conservation law under the popular fractional flow formulation (Chen et al. 2006). The elliptic pressure equation is obtained by summing the governing equations of the phases

$$\nabla \cdot \mathbf{u}_T = q_T,$$  \hspace{1cm} (2.12)

where \( \mathbf{u}_T \) is the total velocity

$$\mathbf{u}_T = \mathbf{u}_o + \mathbf{u}_w = -k \lambda_T \nabla p - k(\lambda_o \rho_o + \lambda_w \rho_w) g \nabla h.$$  \hspace{1cm} (2.13)

where the total mobility is defined as \( \lambda_T = \sum \alpha \lambda_\alpha \). From here on we let \( S \equiv S_w \), and rewrite the water phase velocity in terms of the total velocity as

$$\mathbf{u}_w = V_w(S) \mathbf{u}_T - G(S) C_g,$$  \hspace{1cm} (2.14)

where \( V_w(S) \) and \( G(S) \) are the viscous and gravity part, respectively

$$V_w = \frac{M k_{rw}}{k_{ro} + M k_{rw}},$$  \hspace{1cm} (2.15)

and,

$$G = \frac{M k_{ro} k_{rw}}{k_{ro} + M k_{rw}},$$  \hspace{1cm} (2.16)

where \( M \) is the viscosity ratio, \( \mu_o/\mu_w \). The dimensionless gravity number \( C_g \) is

$$C_g = \frac{k g (\rho_w - \rho_o)}{\mu_o} \nabla h.$$  \hspace{1cm} (2.17)

The non-convex fractional flow function may also become non-monotonic in the presence of buoyancy forces. The water transport equation is finally written as

$$\phi \frac{\partial S}{\partial t} + \nabla \cdot (V_w(S) \mathbf{u}_T - G(S) C_g) = q_w,$$  \hspace{1cm} (2.18)
In 1D, the above equation can be discretized using the finite-volume formulation as

\[
(S_{i}^{n+1} - S_{i}^{n}) + \frac{\Delta t}{\phi \Delta x} (F_{i,i+1}^{n+1} - F_{i-1,i}^{n+1}) = 0. \tag{2.19}
\]

where \(\Delta t\) is timestep and \(\Delta x\) is cell size. Here we define \(S_{i}\) as the upstream state with respect to the total velocity \(u_{T}\), and \(S_{j}\) as the downstream state. For example, as shown in Fig. 2.1, the upstream for \(F_{ij}\) is cell \(i\) if the direction of total velocity is from cell \(i\) to \(j\) \((u_{T} > 0)\). In this work, we always take the total velocity to be positive.

![Figure 2.1: Flux between two neighboring cells](image)

Figure 2.1: Flux between two neighboring cells

It has been shown that nonlinear properties of the numerical flux can have large impact on the convergence behavior of the Newton-based iterative process (Wang and Tchelepi 2013). In this section we review some existing numerical flux schemes, including the recently proposed hybrid upwinding (HU) scheme.

2.3.1 Review of the existing numerical flux schemes

**Phase-Potential Upwinding (PPU).**

In the PPU approach, the upstream direction of a fluid phase is determined according to the gradient of its potential across the interface between two computational cells. Recent studies have revealed that the non-differentiability in the PPU flux caused by the upstream direction switching could be a major cause of nonlinear convergence difficulties. The kink changes the curvature of the numerical flux abruptly, creating oscillations in Newton iterations that may lead to convergence failure.
In PPU, the phase relative permeabilities (or mobilities) at the cell interface \((ij)\) are evaluated as,

\[
k_{\alpha,ij} = \begin{cases} 
  k_{\alpha}(S_i), & \Delta p_{ij} + \rho_{\alpha} g \Delta h_{ij} > 0 \\
  k_{\alpha}(S_j), & \text{otherwise}
\end{cases} \quad \alpha = w, o. 
\] (2.20)

From Eq. (2.20), we can rewrite the upstream conditions in terms of \(u_T\) as,

\[
k_{rw,ij} = \begin{cases} 
  k_{rw}(S_i), & u_T - C_g k_{ro} > 0 \\
  k_{rw}(S_j), & \text{otherwise}
\end{cases}
\]  
\[
k_{ro,ij} = \begin{cases} 
  k_{ro}(S_i), & u_T + C_g M k_{rw} > 0 \\
  k_{ro}(S_j), & \text{otherwise}
\end{cases} 
\]  

(2.21)

Eq. (2.21) does not explicitly define the upstream direction of \(k_{\alpha}\). Brenier and Jaffre (1991) showed how to explicitly determine the upstream criteria,

\[
k_{rw,ij} = \begin{cases} 
  k_{rw}(S_i), & \theta_w > 0 \\
  k_{rw}(S_j), & \text{otherwise}
\end{cases} \quad \] (2.22)

where

\[
\theta_w = u_T - C_g k_{ro}(S_i) 
\] (2.23)

and,

\[
k_{ro,ij} = \begin{cases} 
  k_{ro}(S_i), & \theta_o > 0 \\
  k_{ro}(S_j), & \text{otherwise}
\end{cases} \quad \] (2.24)

where

\[
\theta_o = u_T + C_g M k_{rw}(S_i) 
\] (2.25)

In the transport iterations, because the total-velocity field is fixed, flow reversal from co-current to counter-current at a cell interface depends only on the saturation change in the upwind cell. From Eqs. (2.23) and (2.25), if \(C_g > 0\) (updip), \(\theta_o\) is always positive, and
subsequently,

\[
\begin{cases}
  k_{rw,ij} = k_{rw}(S_i) \text{ and } k_{ro,ij} = k_{ro}(S_i), & 0 \leq \theta_w \leq \theta_o \\
  k_{rw,ij} = k_{rw}(S_j) \text{ and } k_{ro,ij} = k_{ro}(S_i), & \theta_w \leq 0 \leq \theta_o
\end{cases}
\]  

(2.26)

If \(C_g < 0\) (downdip), now \(\theta_w\) is always positive, and thus,

\[
\begin{cases}
  k_{rw,ij} = k_{rw}(S_i) \text{ and } k_{ro,ij} = k_{ro}(S_i), & \theta_w \leq 0 \leq \theta_o \\
  k_{rw,ij} = k_{rw}(S_i) \text{ and } k_{ro,ij} = k_{ro}(S_j), & \theta_o \leq 0 \leq \theta_w
\end{cases}
\]  

(2.27)

**Hybrid Upwinding (HU).**

Lee et al. (2015) proposed a consistent, monotone, and differentiable numerical flux scheme called Hybrid Upwinding (HU) for the two-phase transport. In HU, the phase flux is divided into two parts based on the driving force. The viscous part \(V_w\) in Eq. (2.14), which is always co-current, is upwinded based on the direction of the total-velocity,

\[
S_{ij}^U = \begin{cases} 
  S_i, & \text{if } u_T > 0 \\
  S_j, & \text{if } u_T \leq 0
\end{cases}
\]  

(2.28)

The buoyancy-driven flux across an interface is always counter-current and is upwinded such that the heavier fluid goes downward and the lighter fluid goes upward,

\[
\begin{cases}
  S_{wij}^G = S_j \text{ and } S_{o,ij}^G = 1 - S_i, & \text{if } C_g \geq 0 \\
  S_{wij}^G = S_i \text{ and } S_{o,ij}^G = 1 - S_j, & \text{if } C_g < 0
\end{cases}
\]  

(2.29)

The final formulae of HU are

\[
V_{w,ij} = V_w(S_{ij}^U),
\]  

(2.30)

and,

\[
G_{ij} = G(S_{wij}^G, S_{o,ij}^G).
\]  

(2.31)

The HU scheme is extended to the three-phase case by Lee and Efendiev (2016), and to the coupled flow and transport with multiple phases by the recent works (Hamon and

**Godunov scheme.**

The Godunov flux applies an exact Riemann solver for the scalar hyperbolic conservation laws at the cell interfaces (LeVeque 2002). Compared with PPU, the Godunov flux is rarely used in reservoir simulation, because it is generally more difficult to locate potential sonic points than it is to employ the PPU upwinding criteria during a fully-implicit solution process. Also the Godunov flux is not $C^1$-continuous with respect to $S$ at sonic points. In the scheme, the total-flux function is defined as

$$f(S) = u_w(S)$$

(2.32)

and the numerical flux at the interface is given by

$$F(S_i, S_j) = \begin{cases} 
\min_{S \in [S_i, S_j]} f(S) & \text{for } S_i \leq S_j \\
\max_{S \in [S_j, S_i]} f(S) & \text{for } S_i \geq S_j 
\end{cases}$$

(2.33)

2.3.2 The proposed $C^1$-PPU scheme

Non-differentiabilty in the discrete governing equations can have dramatic effects on the nonlinear convergence behavior. Recently proposed methods address improved smoothness of the numerical flux (Lee et al. 2015). Our objective is to devise and analyze an alternative numerical flux scheme that allows a smooth variation between the co-current/counter-current flow regimes as well as an optimal balance between the properties of accuracy and nonlinearity. The proposed $C^1$-PPU scheme involves a novel use of the flux limiter concept from the context of high-resolution methods. Flux limiters have the effect of limiting the solution gradient in order to prevent spurious oscillations that would otherwise occur with high-order spatial discretization schemes in the presence of shocks or discontinuities. One can combine a low-order flux with a higher-order flux to obtain a flux-limiter method, in the
form of (LeVeque 2002)

\[ F_{ij} = f_{ij}^{\text{low}} + \Phi(r) \left( f_{ij}^{\text{high}} - f_{ij}^{\text{low}} \right). \]  

(2.34)

where \( \Phi(r) \) is a flux limiter. Generally, any two fluxes can be combined to construct a scheme that switches between them, according to the flux limiter concept. Notice that the PPU scheme in Eq. (2.21) is nothing more than a switching criterion; thus it can also be represented in the form of Eq. (2.34). For \( C_g > 0 \), the PPU flux can be rewritten as

\[ F_{ij} = \theta_w [V_{w,i} + \Phi(-\theta_w) (V_{w,j} - V_{w,i})], \]  

(2.35)

where \( V_{w,i} \) and \( V_{w,j} \) are evaluated according to the sign of \( \theta_w \) based on the upwinding scheme shown in Eq. (2.26)

\[ V_{w,i} = \frac{Mk_{rw}(S_i)}{k_{ro}(S_i) + Mk_{rw}(S_i)}, \]  

(2.36)

\[ V_{w,j} = \frac{Mk_{rw}(S_j)}{k_{ro}(S_i) + Mk_{rw}(S_j)}. \]  

(2.37)

\( \Phi(-\theta_w) \) is a simple switching function,

\[ \Phi(-\theta_w) = \begin{cases} 
1 & \text{for } -\theta_w > 0 \\
0 & \text{for } -\theta_w \leq 0 
\end{cases}. \]  

(2.38)

In order to obtain a continuously differentiable flux function, now we first transform Eq. (2.38) into

\[ \Phi(-\theta_w) = \max (-\theta_w, 0) / (-\theta_w), \]  

(2.39)

Next, we replace the non-differentiable function, \( \max (x, 0) \), with a smooth alternative

\[ M_{\mu}(\epsilon, x) = x + \epsilon \log \left( 1 + e^{-x/\epsilon} \right), \]  

(2.40)

where the smoothing coefficient \( \epsilon > 0 \). The final formulae for the \( C^1 \)-continuous PPU flux
can be expressed as

\[
F_{ij}^{C1}(S_i, S_j) = \theta_w [V_{w,i} - M_\mu(\epsilon, -\theta_w)/(\theta_w (V_{w,j} - V_{w,i}))].
\]  

(2.41)

\[
= \theta_w V_{w,i} - M_\mu(\epsilon, -\theta_w) (V_{w,j} - V_{w,i})
\]

Clearly, the C1-PPU flux has differentiability, thanks to the smoothing function. Next we investigate the consistency and monotonicity properties of C1-PPU, which are critical for the analysis of a finite-volume scheme applied to the hyperbolic conservation equations. For the consistency, the following proposition can be easily verified,

**Proposition 2.3.1 (consistency).** The numerical flux of C1-PPU defined in Eq. (2.41) for the scalar conservation law is consistent, i.e.

\[
F_{ij}^{C1}(S, S) = \theta_w V_w(S) = u_w(S).
\]

(2.42)

### 2.3.3 Loss of monotonicity and a fix for C1-PPU

In order for a numerical flux scheme to converge to the entropy solution of the nonlinear scalar conservation laws under implicit time discretization, the scheme has to satisfy the monotonic property, which is introduced through the following definition,

**Definition 2.3.1 (monotonicity).** For all \(i \in \{1, ..., N\}\) and \(j \in \text{adj}(i)\), the numerical flux of phase \(\alpha\), \(F_{\alpha,ij}\), is monotone with respect to its own saturation if, for a constant \(u_T\), \(F_{\alpha,ij}\) is nondecreasing in the \(\alpha\)th component of the first argument, and nonincreasing in the \(\alpha\)th component of the second argument,

\[
\frac{\partial F_{\alpha,ij}}{\partial S_{\alpha,i}} \geq 0 \quad \text{and} \quad \frac{\partial F_{\alpha,ij}}{\partial S_{\alpha,j}} \leq 0
\]

(2.43)

The PPU numerical flux satisfies the property for two- and three-phase transport
(Brenier and Jaffre 1991). Kwok and Tchelepi (2008) present the result proving that implicit monotone schemes applied to scalar hyperbolic conservation laws (two-phase case) produce a unique solution for bounded initial data,

**Theorem 2.3.1** (existence and uniqueness). Assume that \( u_T \) is constant and the initial condition \( \{S_i^0\}_{i \in \{1, \ldots, N\}} \) is bounded. \( F_{ij} \) is monotone and locally Lipschitz continuous. Then the finite-volume scheme defined in Eq. (2.19) has a unique bounded solution \( \{S_i^{n+1}\}_{i \in \{1, \ldots, N\}} \).

Moreover, this bounded solution satisfies the estimate,

\[
\inf_{j \in \{1, \ldots, N\}} S_j^n \leq S_i^{n+1} \leq \sup_{j \in \{1, \ldots, N\}} S_j^n \quad i \in \{1, \ldots, N\}
\]  

(2.44)

Eymard et al. (1998) provide a similar result on the existence and uniqueness of the approximate solution. Also, the implicit monotone scheme will converge to the entropy solution of the scalar conservation law (Eq. (2.18)) upon refinement (Crandall and Majda 1980), if the assumptions of Theorem 2.3.1 are satisfied. It should be noted that the estimate stated in Eq. (2.44) does not apply to the three-phase case, in which the mathematical model becomes a system of coupled conservation laws. Even when the initial condition is monotone, the analytical solution of a three-phase transport problem may evolve into a nonmonotone saturation profile. Specifically, considering a domain \( \Omega = [0, 1] \) and an initial saturation profile \( S_\alpha(\cdot, 0) \) such that \( S_R \leq S_\alpha(x, 0) \leq S_L \) for all \( x \in \Omega \), there may be a time \( t_0 > 0 \) sufficiently large and \( x_0 \in \Omega \) such that \( S_\alpha(x_0, t_0) > S_L \) or \( S_\alpha(x_0, t_0) < S_R \). This feature of the three-phase model, caused by the formation of an oil bank, is supported by core-flood experiments. Thus, Theorem 2.3.1 is irrelevant for the numerical scheme applied to the three-phase case (Hamon and Tchelepi 2016).

We examine the numerical fluxes of the different upwinding schemes. In the following examples, we assume that the total-velocity and the gravity number are constant: \( u_T = 0.01 \) and \( C_g = 0.05 \). The viscosity ratio is \( M = 5 \), and quadratic relative-permeability functions are used: \( k_{rw} = S^2, k_{ro} = (1 - S)^2 \). The smoothing coefficient \( \epsilon \) in Eq. (2.40) is set to 0.005.
The numerical fluxes are plotted against the left cell saturation $S_i$. **Fig. 2.2(a)** shows the results for $S_j = 0.0$ and **Fig. 2.2(b)** for $S_j = 0.01$. We can clearly see that the monotonic flux property is violated by the C1-PPU scheme.

![Figure 2.2(a): Numerical fluxes with respect to the left cell saturation $S_i$](image1)

![Figure 2.2(b): Numerical fluxes with respect to the left cell saturation $S_i$](image2)

To ensure the monotonic flux, we introduce a constraint coefficient $\alpha$ within the smoothing max function

$$M_\mu(\epsilon, -\theta_w) = -\theta_w + \gamma \log \left( 1 + e^{\theta_w/\epsilon} \right),$$  \hspace{1cm} (2.45)
Through the following physically motivated constraint

\[
F_{ij}^{C1} (S_i = 1, S_j = 0) = F_{ij}^{PPU} (S_i = 1, S_j = 0) = u_T,
\]

(2.46)

where \( F_{ij}^{PPU} \) is the PPU flux. We may obtain \( \gamma \) as

\[
\gamma = \frac{u_T}{\log(1 + e^{u_T/\epsilon})}.
\]

(2.47)

In this way the end points of the flux function are restricted and now we can verify that the modified C1-PPU flux satisfies the monotonic property,

**Proposition 2.3.2** (monotonicity). Assume that the mobility of phase \( \alpha \) is increasing with respect to its saturation and decreasing with respect to the saturation of the other phases. Then the C1-PPU numerical flux defined in Eqs. (2.41) and (2.45) is a monotone function of the saturation \( S \) (Definition 3.4.1).

**Proof.** The sign of the partial derivatives of the numerical flux is determined to prove this proposition. Without loss of generality, we assume \( u_T > 0 \) and \( C_g > 0 \). We rewrite Eq. (2.41) as,

\[
F_{ij}^{C1} (S_i, S_j) = (\theta_w + M_\mu) V_{w,i} - M_\mu V_{w,j}
= A_m V_{w,i} - M_\mu V_{w,j}
\]

(2.48)

where \( M_\mu \) is computed by Eq. (2.45), and,

\[
A_m = \gamma \log \left(1 + e^{\theta_w/\epsilon}\right)
\]

(2.49)

We first deal with the sign of \( (A_m V_{w,i}) \). It can be easily verified that,

\[
\frac{\partial A_m}{\partial S_i} \geq 0 , \quad \frac{\partial V_{w,i}}{\partial S_i} \geq 0 , \quad A_m \geq 0 , \quad V_{w,i} \geq 0
\]

(2.50)
These allow us to obtain,

\[ \frac{\partial (A_m V_{w,i})}{\partial S_i} \geq 0 , \quad \frac{\partial (A_m V_{w,i})}{\partial S_j} = 0 \]  

(2.51)

Now we determine the \((M\mu V_{w,j})\) part,

\[ M\mu V_{w,j} = M k_{rw}(S_j) \frac{M\mu}{k_{ro}(S_i) + M k_{rw}(S_j)} \]  

(2.52)

Because we have,

\[ M\mu(S_i = 1) = 0 \quad \text{and} \quad \frac{\partial M\mu}{\partial S_i} \leq 0 \]  

(2.53)

We deduce \(M\mu \geq 0\). Then the partial derivative with respect to \(S_j\) is,

\[ -\frac{\partial (M\mu V_{w,j})}{\partial S_j} = -M\mu \frac{\partial V_{w,j}}{\partial S_j} \leq 0 \]  

(2.54)

Thus \(F^{C1}_{ij}(S_i, S_j)\) is nonincreasing with respect to the second argument. The partial derivative with respect to \(S_i\) is,

\[ \frac{\partial (M\mu V_{w,j})}{\partial S_i} = C_m \left[ \frac{\partial M\mu}{\partial S_i} (k_{ro}(S_i) + M k_{rw}(S_j)) - M\mu \frac{\partial k_{ro}(S_i)}{\partial S_i} \right] \]  

(2.55)

where,

\[ C_m = \frac{M k_{rw}(S_j)}{(k_{ro}(S_i) + M k_{rw}(S_j))^2} \geq 0 \]  

(2.56)

We can deduce that,

\[ \frac{\partial M\mu}{\partial S_i} (k_{ro}(S_i) + M k_{rw}(S_j)) - M\mu \frac{\partial k_{ro}(S_i)}{\partial S_i} \leq 0 , \quad -\frac{\partial (M\mu V_{w,j})}{\partial S_i} \geq 0 \]  

(2.57)

Thus \(F^{C1}_{ij}(S_i, S_j)\) is nondecreasing with respect to the first argument.

\[ \square \]

Fig. 2.8 plots the \((-M\mu V_{w,j})\) part in Eq. (2.48) against \(S_i\) with \(\epsilon = 0.03\). This term is clearly a nondecreasing function of \(S_i\). In Fig. 2.4 the modified C1-PPU numerical fluxes
Figure 2.3: Monotonicity of the term in the C1-PPU flux function from Eq. (2.45) appear with different smoothing coefficients for $S_j = 0.1$. Fig. 2.5 shows the results for $S_j = 0.0$ and $\epsilon = 0.01$. We also examine the numerical fluxes for buoyancy- ($C_g = 0.2$) and viscous-dominated ($u_T = 0.1$) scenarios while the other parameters remain unchanged. The results for the buoyancy ($C_g = 0.2$, $\epsilon = 0.01$) and viscous ($u_T = 0.1$, $\epsilon = 0.03$) cases are shown in Figs. 2.6 and 2.7 respectively. From Fig. 2.6 we can
clearly see that the C1-PPU flux has less scalar nonlinearity than HU. The increase in the nonlinearity will inevitably cause a negative impact on the iterative solution performance. It is also observed from the results that C1-PPU has higher accuracy than HU, and is comparable to the classical PPU scheme.

The proposed C1-PPU scheme is still well-defined when $C_g < 0$. In such case, the flux for the oil phase can be first computed by a similar formula as Eq. (2.41)

$$F_{o,ij} = \theta_o V_{o,i} - M_\mu(\epsilon, -\theta_o) (V_{o,j} - V_{o,i}),$$  \hspace{1cm} (2.58)

where $V_{o,i}$ and $V_{o,j}$ are evaluated based on [2.27]

$$V_{o,i} = \frac{k_{ro}(S_i)}{k_{ro}(S_i) + M k_{rw}(S_i)},$$ \hspace{1cm} (2.59)

$$V_{o,j} = \frac{k_{ro}(S_j)}{k_{ro}(S_j) + M k_{rw}(S_i)}.$$ \hspace{1cm} (2.60)

Then the water flux is simply computed as $F_{ij} = u_T - F_{o,ij}$. The monotonicity of the
Figure 2.6: Numerical fluxes for the buoyancy-dominated case with $C_g = 0.2$, $\epsilon = 0.01$

C1-PPU flux for $C_g < 0$ can be proved by a similar procedure as presented in Proposition 2.3.2. The sign of the partial derivatives of $F_{i,j}$ will be first determined, and then take the opposite to obtain the sign for $F_{ij}$. The numerical fluxes for the case with $u_T = 0.01$, $M = 5$, $C_g = -0.05$, $S_j = 0.9$ and $\epsilon = 0.01$ are shown in Fig. 2.8.
2.3.4 Convergence ratio

The scalar nonlinearity also can be investigated from the aspect of convergence ratio. The Kantorovich theorem (Ortega and Rheinboldt 1970) provides a sufficient condition for convergence of the Newton iterations. The theory states that if the residual $R(S)$ in Eq. (2.61) is a $C^2$ function of the solution $S$, then Newton’s method is guaranteed to converge if the convergence ratio $|R(S)R''(S)|/|R'(S)|^2 < 1$ is maintained locally. A convergence ratio less than unity indicates that it is now in the contraction region around the root, and the

Figure 2.7: Numerical fluxes for the viscous-dominated case with $u_T = 0.1$, $\epsilon = 0.03$
iterations will converge (Wang and Tchelepi 2013).

Consider a single cell problem with immiscible two-phase transport. The saturations, $S_L$ and $S_R$, are the left and right boundary conditions. The residual form of the conservation law can be written as

$$R(S^{n+1}) = (S^{n+1} - S^n) + \frac{\Delta t}{\Delta x} (F_R^{n+1} - F_L^{n+1}),$$  \hspace{1cm} (2.61)

where the initial condition is $S^n = 0$. The derivatives of the residual are

$$R' = \frac{dR}{dS^{n+1}} = 1 + \frac{\Delta t}{\Delta x} \left( \frac{\partial F_R(S^{n+1}; S_R)}{\partial S^{n+1}} - \frac{\partial F_L(S_L; S^{n+1})}{\partial S^{n+1}} \right),$$  \hspace{1cm} (2.62)

$$R'' = \frac{d^2R}{d(S^{n+1})^2} = \frac{\Delta t}{\Delta x} \left( \frac{\partial^2 F_R(S^{n+1}; S_R)}{\partial (S^{n+1})^2} - \frac{\partial^2 F_L(S_L; S^{n+1})}{\partial (S^{n+1})^2} \right).$$  \hspace{1cm} (2.63)

We compare the convergence ratios of the different numerical fluxes. The boundary conditions are set to $S_L = 0.5$ and $S_R = 0.9$. We take $u_T = 1$, $M = 1$ and $C_g = -10$. The ratio $\frac{\Delta t}{\Delta x}$ is 2 and $\epsilon = 1$. In this scenario, buoyancy forces are more dominant than viscous forces. The convergence ratios are plotted versus the saturation in Fig. 2.9 From the
figure we can see that the convergence ratio of PPU is quite different between the two sides of the unit-flux point due to the counter-current flow, while the other two schemes with $C^1$ continuity do not exhibit this property. It can also be seen that the range of saturation values where the convergence ratio is below unity (the contraction region) for HU is much smaller than the C1-PPU scheme, which indicates less scalar nonlinearity inherent in C1-PPU for this case.

![Convergence ratios of the different numerical fluxes](image)

**Figure 2.9: Convergence ratios of the different numerical fluxes**

The trust-region Newton scheme employs a strategy that does not allow two successive saturation updates to reside on opposite sides of the unit-flux point, in order to overcome the convergence difficulty associated with the counter-current flow (Wang and Tchelepi 2013; Li and Tchelepi 2015). For the continuously differentiable HU and C1-PPU schemes, however, this chopping based Newton method is not necessary because there is no kink in the residual around the unit flux point.

### 2.3.5 Adaptive smoothing coefficient

An adaptive strategy is proposed to properly choose the smoothing coefficient in the
C1-PPU scheme. Eq. (2.41) is first reformulated as,

\[
F_{ij}^{C1}(S_i, S_j) = \theta_w V_{w,i} - \max(-\theta_w, 0)(V_{w,j} - V_{w,i}) \\
- (M_\mu(\epsilon, -\theta_w) - \max(-\theta_w, 0))(V_{w,j} - V_{w,i})
\]  

(2.64)

where the C1-PPU flux is split into two parts: one recovers the original PPU flux; the other represents the error term introduced through the smoothing operation. As will be shown in the next section, the difference between the max function and its smooth alternative is bounded by a constant, which depends on a fixed smoothing coefficient \( \epsilon \). Therefore, the upper bound of the flux in the domain can be estimated first for a specific simulation case. Then the adaptive smoothing coefficient can be expressed as,

\[
\epsilon = \kappa \max |F_{ij}^{PPU}|
\]

(2.65)

where \( \kappa \) is a factor controlling the maximum error introduced in the flux magnitude by the smoothing function. In this work we find that \( \kappa = 0.2 \) can be very effective for obtaining the balance between the smoothness and accuracy of the numerical flux. We consider the case with \( u_T = 0.01, M = 5 \) and \( S_j = 0.1 \). The numerical fluxes for \( C_g = 0.05 \) and \( C_g = 0.5 \) are plotted in Fig. 2.10. The adaptive smoothing coefficients computed through Eq. (2.65) are \( \epsilon = 0.006 \) and \( \epsilon = 0.08 \), respectively.

### 2.4 C1-PPU for coupled multiphase flow and transport

In this section we propose a generalization of C1-PPU to an arbitrary number of phases. We intend to directly deal with the mass conservation equations (Eq. (2.1)) for the coupled flow and transport in multiple dimensions. To develop the generalized schemes based on the upwinding criteria in Eq. (2.20), we first define the phase potential difference between two adjacent cells

\[
\Delta \varphi_{i,j} = \Delta p_{ij} + \rho_0 g \Delta h_{ij}.
\]

(2.66)
Figure 2.10: Numerical fluxes computed using the adaptive smoothing formula

The two-point interface flux $F^{PPU}_{\alpha,ij} (\Delta p_{ij}, S_i, S_j)$ for each phase is written as

$$F^{PPU}_{\alpha,ij} (\Delta p_{ij}, S_i, S_j) = T_{ij} \lambda^{PPU}_{\alpha,ij} \Delta \varphi_{\alpha,ij}. \quad (2.67)$$

The generalized C1-PPU flux $F^{C1}_{\alpha,ij}$ can be expressed in a similar form as Eq. (2.41)

$$F^{C1}_{\alpha,ij} = T_{ij} \left( \Delta \varphi_{\alpha,ij} \lambda_{\alpha}(S_i) - M_{\mu}(\epsilon, -\Delta \varphi_{\alpha,ij}) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \right). \quad (2.68)$$
where \( S_i = \{ S_{k,i} \}_{k \in \{1, \ldots, n_p\}} \); and we drop the superscript \((n + 1)\) of the current time level in the flux term. The smoothing approximation function \( M_\mu(\epsilon, x) \) of \( H(x) = \max(x, 0) \) is constructed such that for any \( \epsilon > 0 \), \( M_\mu(\epsilon, x) \) is continuously differentiable and satisfies,

\[
\| M_\mu(\epsilon, x) - H(x) \| \to 0 \quad \text{as} \quad \epsilon \to 0^+, \tag{2.69}
\]

Here we present two versions of the smoothing max function

\[
M_{\mu 1}(\epsilon, x) = x + \epsilon \log \left( 1 + e^{-x/\epsilon} \right), \tag{2.70}
\]

and

\[
M_{\mu 2}(\epsilon, x) = 0.5(x + \sqrt{x^2 + \epsilon^2}). \tag{2.71}
\]

These two versions are chosen for the reason that they are always positive. As will be shown later, the positivity of the smoothing functions plays a key role in the proof of the saturation estimate for the C1-PPU scheme. We also introduce a boundedness property of the smoothing functions, which is critical to the pressure estimate of the scheme,

**Proposition 2.4.1** (boundedness). When \( \epsilon > 0 \), there exists a constant \( \eta > 0 \) such that,

\[
\| M_\mu(\epsilon, x) - H(x) \| \leq \eta \epsilon \tag{2.72}
\]

**Proof.** First consider \( M_{\mu 1}(\epsilon, x) \). For \( x \geq 0 \),

\[
M_{\mu 1}(\epsilon, x) - H(x) = \epsilon \log \left( 1 + e^{-x/\epsilon} \right) \leq \epsilon \log (1 + 1) = \epsilon \log 2
\]

37
and for $x < 0$,

$$
M_{\mu_1}(\epsilon, x) - H(x) = x + \epsilon \log \left(1 + e^{-x/\epsilon}\right) \\
\leq \log e^x + \epsilon \log \left(2e^{-x/\epsilon}\right) = \epsilon \log 2
$$

(2.74)

For $M_{\mu_2}(\epsilon, x)$, with $x \geq 0$,

$$
M_{\mu_2}(\epsilon, x) - H(x) = 0.5 \left(x + \sqrt{x^2 + \epsilon^2}\right) - x \\
\leq 0.5 \left(x + \sqrt{(x + \epsilon)^2}\right) - x = 0.5 \epsilon
$$

(2.75)

and for $x < 0$,

$$
M_{\mu_2}(\epsilon, x) - H(x) = 0.5 \left(x + \sqrt{x^2 + \epsilon^2}\right) \\
\leq 0.5 \left(x + \sqrt{(x - \epsilon)^2}\right) = 0.5 \epsilon
$$

(2.76)

Thus $\eta_1 = \log 2$ and $\eta_2 = 0.5$. Also we can easily verify that,

$$
M_{\mu_1}(\epsilon, x) - H(x) \geq 0 \quad \text{and} \quad M_{\mu_2}(\epsilon, x) - H(x) \geq 0
$$

(2.77)

We plot $H(x) = \max(x, 0)$ and the smoothing approximation functions $M_{\mu}(\epsilon, x)$ with $\epsilon = 300$ in Fig. 2.11. We also set a case with $S_L = 0.8$, $S_R = 0.2$, $g = 10$, $\Delta h = 0.3048$, $\rho_o = 161$ and $T_{ij} = 9e - 12$. The C1-PPU numerical fluxes based on Eq. (2.71) with different smoothing coefficients are shown in Fig. 2.12.

We now study the mathematical properties of the generalized C1-PPU flux defined by Eq. (2.68). Similarly to Eq. (2.42), we can deduce that the flux is consistent. As stated previously, no proof of convergence to a unique solution is available for the transport problem with three or more fluid phases. Following the similar procedures as presented in the previous works (Enchery et al. 2002; Eymard et al. 2003; Saad and Saad 2013; Hamon and Tchelepi 2016; Hamon et al. 2016), we provide proofs of the saturation and pressure...
estimates, which are then used to show the existence of a solution to the C1-PPU scheme for an arbitrary number of phases. For simplicity, the rock and fluid compressibility is neglected.
here, and Eq. (4.7) becomes,

$$\frac{\phi_i |Q_i|}{\Delta t} (S_{a,i}^{n+1} - S_{a,i}^{n}) + \sum_{j \in \text{adj}(i)} F_{a,i,j}^{n+1} (\Delta p_{ij}, S_i, S_j) = Q_{a,i}^I - Q_{a,i}^P^{n+1}(S_i) \quad (2.78)$$

where $\alpha \in \{1, ..., n_p\}$, $i \in \{1, ..., N\}$, $n \in \{0, ..., M-1\}$, $S_i = \{S_{k,i}\}_{k \in \{1, ..., n_p\}}$ and the initial condition $S_{a,i}^0 = S_{a,i}^{\text{init}}$. $Q_{a}^I$ and $Q_{a}^P(S_i)$ are the fixed positive well terms for injection and production, respectively.

2.4.1 Saturation estimate

A physically based maximum principle is provided, guaranteeing that saturations remain between physical bounds,

**Proposition 2.4.2** (physically based maximum principle). It is assumed that the relative permeability of phase $\alpha$ is positive, with $k_{r\alpha}(S_1, ..., S_{n_p}) = 0$ whenever $S_\alpha \leq 0$. Consider the finite-volume discretization with the C1-PPU flux defined by Eqs. (2.68) and (2.78). An initial condition $(p^{\text{init}}, S^{\text{init}})$ is specified with $0 \leq S_{a,i}^{\text{init}} \leq 1$ for all $\alpha \in \{1, ..., n_p\}$, and $i \in \{1, ..., N\}$. Suppose that $(p, S)$ is a solution to the discretization satisfying the saturation constraint in Eq. (2.2). Then the following physically based maximum principle applies to $n \in \{1, ..., M\}$,

$$0 \leq S_{a,i}^n \leq 1 \quad (2.79)$$

**Proof.** Assume that the physical bounds given in Eq. (2.79) are valid for $n \in \{1, ..., n_c\}$ with $n_c \leq M - 1$. Suppose two integers $\alpha_c$ and $i_c$ such that $S_{\alpha_c,i_c}^{n+1} < 0$. The discrete equation for control volume $i_c$ and phase $\alpha_c$ can be reformulated as,

$$S_{\alpha_c,i_c}^{n} = S_{\alpha_c,i_c}^{n+1} + \frac{\Delta t}{\phi_{i_c} |\Omega_{i_c}|} \left( \sum_{j \in \text{adj}(i_c)} F_{\alpha_c,i_c,j}^{n+1} - (Q_{\alpha_c,i_c}^I - Q_{\alpha_c,i_c}^P^{n+1}(S_{i_c})) \right) \quad (2.80)$$

$$< \frac{\Delta t}{\phi_{i_c} |\Omega_{i_c}|} \left( \sum_{j \in \text{adj}(i_c)} F_{\alpha_c,i_c,j}^{n+1} - (Q_{\alpha_c,i_c}^I - Q_{\alpha_c,i_c}^P^{n+1}(S_{i_c})) \right).$$
We first consider the flux term in Eq. (2.80),

\[
\sum_{j \in \text{adj}(i_c)} F_{\alpha,ic,j}^{n+1} = \sum_{j \in \text{adj}(i_c)} T_{ic,j} \left( \Delta \varphi_{\alpha,ic,j} \lambda_{\alpha}(S_{ic}) - M_\mu (\lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_{ic})) \right) \tag{2.81}
\]

According to the assumption on phase relative permeability, \( S_{\alpha,ic} < 0 \) implies \( \lambda_{\alpha}(S_{ic}) = 0 \). Thanks to the positivity of the smoothing functions \( (M_\mu > 0) \), we can obtain,

\[
\sum_{j \in \text{adj}(i_c)} F_{\alpha,ic,j}^{n+1} = \sum_{j \in \text{adj}(i_c)} T_{ic,j} \left( -M_\mu \lambda_{\alpha}(S_j) \right) \leq 0 \tag{2.82}
\]

For the well term in Eq. (2.80), \( S_{\alpha,ic} < 0 \) implies \( Q_{\alpha,ic}^{P,n+1}(S_{ic}) = 0 \), which leads to,

\[
- \left( Q_{\alpha,ic}^{I,n+1} - Q_{\alpha,ic}^{P,n+1}(S_{ic}) \right) = -Q_{\alpha,ic}^{I} \leq 0 \tag{2.83}
\]

Through Eqs. (2.82) and (2.83), we obtain \( S_{\alpha,ic}^{n+1} < 0 \), which is contradictory to the initial assumption of this proof. Now suppose that there exists \( \alpha_c \) and \( i_c \) such that \( S_{\alpha,ic}^{n+1} > 1 \). The saturation constraint in Eq. (2.2) gives,

\[
\sum_{m \neq \alpha_c} S_{m,ic}^{n+1} = 1 - S_{\alpha,ic}^{n+1} < 0 \tag{2.84}
\]

Therefore, there exists \( \alpha_d \in \{1, \ldots, n_p\} \setminus \alpha_c \) such that \( S_{\alpha_d,ic}^{n+1} < 0 \). Based on what we just proved, we obtain \( S_{\alpha,ic}^{n+1} < 0 \), which is again contradictory to the initial assumption. Hence the double inequality in Eq. (2.79) holds at time \( n_c + 1 \), and we obtain the maximum principle for \( n \in \{1, \ldots, M\} \) by induction.

\[\square\]

2.4.2 Pressure estimate

Before proceed to the proof for the pressure estimate, we first recall the total velocity of multiphase flow,

\[
u_T = \sum_\alpha \nu_\alpha = -k \lambda_T \nabla p - kg \nabla h \sum_\alpha \lambda_\alpha \rho_\alpha \tag{2.85}
\]
The sum of the discrete fluxes over all phases is equal to $u_{T,ij}$,

$$\sum_{\alpha} F_{\alpha,ij} = u_{T,ij} \quad (2.86)$$

Next, the C1-PPU flux is rewritten as,

$$F_{\alpha,ij} = T_{ij} \left( \Delta \varphi_{\alpha,ij} \lambda_{\alpha}(S_i) - H(-\Delta \varphi_{\alpha,ij}) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \right)$$

$$- \left( M_{\mu}(\epsilon, -\Delta \varphi_{\alpha,ij}) - H(-\Delta \varphi_{\alpha,ij}) \right) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \right) \quad (2.87)$$

The flux is split into two parts,

$$F_{\alpha,ij} = F_{\alpha,ij}^{PPU} - F_{\alpha,ij}^{DS} \quad (2.88)$$

where the $F_{\alpha,ij}^{PPU}$ part recovers the original PPU flux,

$$F_{\alpha,ij}^{PPU} = T_{ij} \left( \Delta \varphi_{\alpha,ij} \lambda_{\alpha}(S_i) - H(-\Delta \varphi_{\alpha,ij}) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \right) \quad (2.89)$$

and,

$$F_{\alpha,ij}^{DS} = T_{ij} \left( M_{\mu}(\epsilon, -\Delta \varphi_{\alpha,ij}) - H(-\Delta \varphi_{\alpha,ij}) \right) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \quad (2.90)$$

The above formulations are used to find an upper-bound to the squared pressure differences summed over all the cell interfaces for the pressure estimate, which is valid for an arbitrary number of phases.

Proposition 2.4.3 (pressure estimate). Consider the finite-volume discretization with the C1-PPU flux defined by Eqs. (2.68) and (2.78). Suppose that $(p, S)$ is a solution to the discretization. Then there exists $C \in \mathbb{R}^+$ independent of $(p, S)$ such that the following estimate holds for $n \in \{0, ..., M - 1\}$,

$$\sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \leq C \quad (2.91)$$
where the sum in Eq. (2.91) is taken over the \( n_{ij} \) cell interfaces.

**Proof.** We first sum Eq. (2.78) over all phases in cell \( i \) to obtain,

\[
\sum_{j \in \text{adj}(i)} u_{T,ij}^{n+1} (\Delta p_{ij}, S_i, S_j) = Q_{T,i}^{n+1} (S_i) \tag{2.92}
\]

where \( i \in \{1, ..., N\} \). Here the total well term in cell \( i \) is \( Q_{T,i}^{n+1} (S_i) = \sum_{\alpha} (Q_{\alpha,i}^T - Q_{\alpha,i}^{P,n+1} (S_i)) \), and,

\[
u_{T,ij}^{n+1} = u_{PPU,i}^{n+1} - \sum_{\alpha} F_{\text{Diff},ij}^{n+1}\tag{2.93}
\]

where the total velocity in PPU is,

\[
u_{PPU,i}^{n+1} = \sum_{\alpha} T_{ij}^{PPU} \lambda_{\alpha,ij}^{PPU} \left( \Delta p_{ij}^{n+1} + \rho_{\alpha} g \Delta h_{ij} \right) \tag{2.94}
\]

We then multiply Eq. (2.92) by the pressure \( p_{i}^{n+1} \) and sum over all cells to obtain,

\[
\sum_{i} \sum_{j \in \text{adj}(i)} u_{T,ij}^{n+1} (\Delta p_{ij}, S_i, S_j) p_{i}^{n+1} = \sum_{i} Q_{T,i}^{n+1} (S_i) p_{i}^{n+1} \tag{2.95}
\]

Eq. (2.95) can be written as,

\[
E_1 = E_2 + E_3 + E_4 \tag{2.96}
\]

\[
E_1 = \sum_{(ij)} T_{ij}^{PPU} \Delta p_{ij}^{n+1} \tag{2.97}
\]

\[
E_2 = - \sum_{(ij)} T_{ij} g \Delta h_{ij} \Delta p_{ij}^{n+1} \sum_{\alpha} \lambda_{\alpha,ij}^{PPU} \rho_{\alpha} \tag{2.98}
\]

\[
E_3 = \sum_{(ij)} T_{ij} \Delta p_{ij}^{n+1} \sum_{\alpha} (M_{\mu}(\epsilon, -\Delta \varphi_{\alpha,ij}) - H(-\Delta \varphi_{\alpha,ij})) (\lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i)) \tag{2.99}
\]
\[ E_4 = \sum_i Q_{T,i}^{n+1}(S_i)p_i^{n+1} \] (2.100)

The Cauchy-Schwarz inequality is then employed to find an upper bound to \( E_2 \),

\[ |E_2| \leq \left( \sum_{(ij)} T_{ij} (g \Delta h_{ij})^2 \left( \sum_{\alpha} \lambda_{T,ij}^{PPU} \bar{p}_\alpha \right)^2 \right)^{1/2} \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2} \] (2.101)

The upper bound on the total mobility \( \lambda_{T,ij}^{PPU} \leq \tau \) gives,

\[ |E_2| \leq C_1 \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2} \] (2.102)

\[ C_1 = \tau g \max_{(ij)} |\Delta h_{ij}| \bar{p}_k \left( n_{ij} \max_{(ij)} T_{ij} \right)^{1/2} \] (2.103)

where \( \bar{p}_k = \max_{\alpha} \bar{p}_\alpha \). Applying the Cauchy-Schwarz inequality to \( E_3 \), we obtain,

\[ |E_3| \leq \left( \sum_{(ij)} T_{ij} D_S^2 \right)^{1/2} \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2} \] (2.104)

\[ D_S = \sum_{\alpha} \left( M_\mu(\epsilon, -\Delta \varphi_{\alpha,ij}) - H(-\Delta \varphi_{\alpha,ij}) \right) \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \] (2.105)

Through the bounds on the mobility and smoothing function, we have,

\[ \left| \sum_{\alpha} \left( \lambda_{\alpha}(S_j) - \lambda_{\alpha}(S_i) \right) \right| \leq \beta \ , \ M_\mu(\epsilon, x) - H(x) \leq \eta \epsilon \] (2.106)

Then the following inequality can be derived,

\[ |E_3| \leq C_2 \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2} , \ C_2 = \beta \eta \max_{(ij)} \epsilon \left( n_{ij} \max_{(ij)} T_{ij} \right)^{1/2} \] (2.107)
We now obtain an upper bound to \( E_4 \) via the Cauchy-Schwarz inequality,

\[
|E_4| \leq \left( \sum_i \frac{1}{|\Omega_i|} (Q_{T,i}^{n+1}(S_i))^2 \right)^{1/2} \left( \sum_i |\Omega_i| (p_i^{n+1})^2 \right)^{1/2} \tag{2.108}
\]

An upper bound to the pressure sum in Eq. (2.108) is given by the discrete mean Poincaré inequality. Specifically, there exists \( C_P \in \mathbb{R}^+ \) independent of \( p \) and \( S \) such that,

\[
|E_4| \leq C_P \left( \sum_i \frac{1}{|\Omega_i|} (Q_{T,i}^{n+1}(S_i))^2 \right)^{1/2} \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2} \tag{2.109}
\]

\[
\leq C_3 \left( \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \right)^{1/2}, \quad C_3 = C_P \left( \frac{C_4}{\min_j |\Omega_i|} \right)^{1/2}
\]

where \( C_4 \in \mathbb{R}^+ \) is chosen such that \( \sum_i (Q_{T,i}^{n+1}(S_i))^2 \leq C_4 \). Let us now consider the interface \( \Gamma_{ij} \). If the upwind directions (2.20) are the same for all phases (co-current flow), then we have the lower bound on the total mobility,

\[
\lambda_{T,ij}^{PU} \geq \xi \tag{2.110}
\]

Conversely, if there are two phases flowing in opposite directions (counter-current flow), we can deduce that,

\[
(\Delta p_{ij}^{n+1})^2 \leq (\rho_k g \Delta h_{ij})^2 \tag{2.111}
\]

Summing (2.111) over all interfaces, we obtain,

\[
\sum_{(ij)} T_{ij} \xi \mathcal{X}_C (\Delta p_{ij}^{n+1})^2 \leq \sum_{(ij)} T_{ij} \xi (\rho_k g \Delta h_{ij})^2 \leq C_5 \tag{2.112}
\]

\[
C_5 = \xi n_{ij} \max_{(ij)} T_{ij} \left( g \rho_k \max_{(ij)} |\Delta h_{ij}| \right)^2 \tag{2.113}
\]

where \( \mathcal{X}_C = 1 \) if under the counter-current flow condition and 0 otherwise. Moreover, we
have,

\[ \xi \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \leq \sum_{(ij)} T_{ij} (\xi \lambda_C + \lambda_T^{PPU}) (\Delta p_{ij}^{n+1})^2 \leq C_5 + E_1 \] (2.114)

Using the inequality \( xy \leq \frac{x^2}{2} + \frac{y^2}{2} \), and collecting Eqs. (2.96), (2.102), (2.107), (2.109) and (2.114), we obtain,

\[ \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \leq \frac{C_5}{\xi} + \frac{1}{2\xi^2} (C_1 + C_2 + C_3)^2 + \frac{1}{2} \sum_{(ij)} T_{ij} (\Delta p_{ij}^{n+1})^2 \] (2.115)

Finally, we can achieve the estimate (2.91) with,

\[ C = \frac{2C_5}{\xi} + \frac{1}{\xi^2} (C_1 + C_2 + C_3)^2 \] (2.116)

2.4.3 Solution existence

In the following proposition, we state the existence of a solution to the C1-PPU finite-volume scheme for the coupled flow and transport with an arbitrary number of phases. The solution existence is proved along the same line as presented in Hamon and Tchelepi (2016). The proof is based on a topological degree argument and relies on the saturation and pressure estimates derived in Propositions 2.4.2 and 2.4.3. The detailed proof procedure is omitted here for brevity.

**Proposition 2.4.4** (solution existence). There exists at least a solution \((p, S)\) to the finite-volume discretization with the C1-PPU flux defined by Eqs. (2.68) and (2.78).

**Proof.** The solution existence is proved along the same line with the works of Eymard et al. (1998), Enchery et al. (2002), Eymard et al. (2003) and Hamon and Tchelepi (2016). The proof is based on a topological degree argument presented in Deimling (2010). A continuous function \(R(p, S)\) is defined on a suitable space \(\mathcal{X}\) such that the C1-PPU finite-volume scheme can be reformulated as \(R(p, S) = 0\). A homotopy \(H((p, S), \varphi)\), with \(\varphi \in [0, 1]\), is then chosen.
such that \( H((p, S), 1) = R(p, S) \), and that it is simpler to prove the existence of a solution to \( H((p, S), 0) = 0 \). The proof is concluded by using the property of invariance of the topological degree by homotopy. Specifically, consider the space,

\[
X = \mathbb{R}^{1,\ldots,N} \times \mathbb{R}^{1,\ldots,n_p-1} \times \mathbb{R}^{1,\ldots,N} \times \mathbb{R}^{0,\ldots,M}
\]  

and the functions,

\[
R : X \rightarrow X \quad \text{and} \quad H : X \times [0,1] \rightarrow X
\]

with,

\[
H((p, S), \varphi) = (u, v) \quad \text{and} \quad R(p, S) = H((p, S), 1)
\]

Using \( S_i(\varphi) = \varphi S_i^{n+1} + (1 - \varphi)S_{i(\varphi=0)} \) with \( S_{i(\varphi=0)} \in [0,1]^{n_p-1} \) chosen such that for all \( \alpha \in \{1, \ldots, n_p\}, \lambda_\alpha(S_{i(\varphi=0)}) \neq 0 \), the vectors \( u \) and \( v \) are defined as,

\[
v_{0, i}^0 = S_{0, i}^0 - S_{0, i}^{init}
\]

\[
v_{n+1, i} = \frac{\phi_i|\Omega_i|}{\Delta t} \left( S_{n, i}^{n+1} - S_{n, i}^m \right) - \varphi(Q_{n, i}^I - Q_{n, i}^{P,n+1}(S_i))
+ \sum_{j \in \text{adj}(i)} T_{ij} \left( \Delta \varphi_{i,j}(\varphi) \lambda_\alpha(S_i(\varphi)) - M_\mu(\epsilon, -\Delta \varphi_{i,j}(\varphi))(\lambda_\alpha(S_j(\varphi)) - \lambda_\alpha(S_i(\varphi))) \right)
\]

\[
u_{n+1, i} = \frac{\phi_i|\Omega_i|}{\Delta t} \left( S_{n, i}^{n+1} - S_{n, i}^m \right) - \varphi(Q_{n, i}^I - Q_{n, i}^{P,n+1}(S_i))
+ \sum_{j \in \text{adj}(i)} T_{ij} \left( \Delta \varphi_{n,j}(\varphi) \lambda_{n_p}(S_i(\varphi)) - M_\mu(\epsilon, -\Delta \varphi_{n,j}(\varphi))(\lambda_{n_p}(S_j(\varphi)) - \lambda_{n_p}(S_i(\varphi))) \right)
\]

where \( \alpha \in \{1, \ldots, n_p\} \) and \( i \in \{1, \ldots, N\} \).

\[
u_{n+1, i} = \frac{\phi_i|\Omega_i|}{\Delta t} \left( S_{n_p, i}^{n+1} - S_{n_p, i}^m \right) - \varphi(Q_{n_p, i}^I - Q_{n_p, i}^{P,n+1}(S_i))
+ \sum_{j \in \text{adj}(i)} T_{ij} \left( \Delta \varphi_{n_p,j}(\varphi) \lambda_{n_p}(S_i(\varphi)) - M_\mu(\epsilon, -\Delta \varphi_{n_p,j}(\varphi))(\lambda_{n_p}(S_j(\varphi)) - \lambda_{n_p}(S_i(\varphi))) \right)
\]

where \( i \in \{1, \ldots, N - 1\} \) and \( n \in \{0, \ldots, M - 1\} \). \( R \) (resp., \( H \)) is a continuous function of
Consider a ball $B_r$ of radius $r$ in $\mathcal{X}$. The topological degree of $H((p,S),\varphi) = 0$, denoted by $\text{deg}(H((\cdot,\cdot),\varphi),B_r,0)$, is well-defined and independent from $\varphi \in [0,1]$ if there exists $r_0 > 0$ such that $H((p,S),\varphi) \neq 0$ for all $(p,S)$ on the boundary $\partial B_{r_0}$ (Deimling 2010). This is the case here, as from the previous sections, a solution to $H((p,S),\varphi) = 0$ with $\varphi \in [0,1]$ satisfies a priori bounds on pressure and saturation. It is then possible to choose $r_0 > 0$ sufficiently large such that all pairs $(p,S) \in \partial B_{r_0}$ violate these bounds, and hence cannot be solutions to $H((p,S),\varphi) = 0$. The linear problem $H((p,S),0) = 0$ has a unique solution, which implies that $\text{deg}(H((\cdot,\cdot),0),B_r,0) \neq 0$. Since the degree $\text{deg}(H((\cdot,\cdot),\varphi),B_r,0)$ is independent from $\varphi \in [0,1]$, we deduce $\text{deg}(H((\cdot,\cdot),1),B_r,0) = \text{deg}(R,B_r,0) \neq 0$. Thus the C1-PPU finite-volume scheme has at least a solution satisfying Eqs. (2.79) and (2.91). 

The generalized C1-PPU scheme (2.68) for coupled flow and transport problems is derived based on the mass conservation equations, which are different from the fractional flow formulation with separate pressure and saturation equations. The phase flux now depends on the phase potential gradient between the two adjacent cells. Thus, the generalized C1-PPU flux cannot be analyzed with the assumption of a fixed total velocity, and the monotonicity property (Definition 3.4.1) can no longer be proved.

However, it should also be noted that the total velocity is generally a function of space and time in multiple dimensions. Therefore, for the two-phase case we cannot apply the existence and uniqueness results (Theorem 2.3.1) to the fully-implicit method. The analyses only apply to the sequential-implicit methods (SIM), which decouple the system into an elliptic and a hyperbolic subproblem.

In addition, even for the widely used PPU scheme applied to three-phase transport, no proof of convergence to a unique solution under refinement is available. In this work, the convergence and accuracy of the proposed scheme for the coupled problems are investigated.
with numerical examples.

2.4.4 Sequential-implicit solution framework

Sequential-implicit methods (SIM) are also a popular solution strategy to handle the coupled flow and transport in porous media. For each timestep in SIM, there are two inner loops: one for pressure (total-velocity) and one for saturation, and there is an outer loop. For each iteration of the outer loop, the computations proceed as follows: compute the pressure field iteratively to a certain tolerance, update the total-velocity, then compute the saturation iteratively. The phase velocity under the fractional flow formulation is,

$$u_\alpha = \lambda_\alpha u_T + k g \nabla h \sum_m \lambda_m \lambda_\alpha \lambda_T (\rho_\alpha - \rho_m)$$

As shown in the work of Wang (2012), SIM suffers from serious convergence difficulties in the presence of significant buoyancy when the timestep sizes are relatively large. The challenge lies in the fact that the flow directions of the two phases based on the pressure solution may change once the saturation is updated by solving the transport problem. Changes of the phase-flow direction between sequential updates of the pressure and saturation fields can slow down the outer-loop convergence quite significantly.

The proposed C1-PPU scheme can be readily applied in the sequential-implicit solution framework. Instead of dealing with the formulation based on Eq. (2.123), the flux formula given by Eq. (2.68) should be used to approximate the phase velocities and the saturation dependent terms in the total velocity. Then it can be easily shown that for a fixed pressure field, the C1-PPU scheme is monotone with respect to its own saturation. Moreover, C1-PPU allows a smooth variation between the co-current/counter-current flow regimes and thus is expected to resolve the flow reversal issue in SIM.

2.5 1D examples: scalar transport problem

In this section we perform simulation studies to investigate the accuracy and nonlinear convergence of the different numerical flux schemes. We consider a two-phase Buckley-
Leverett problem in 1D with buoyancy effects. Flow is through a domain with unit length, $x \in [0, 1]$. The injection saturation is unity ($S_{\text{inj}} = 1$) at the bottom (left) boundary and fluid is produced from the top (right) boundary. We divide the domain equally into two parts, and assign different initial saturations to each part. For all of the following cases, the smoothing coefficient of C1-PPU is set to $\epsilon = 0.03$.

We first present a viscous-dominated case with $u_T = 0.1$, $M = 5$ and $C_g = 0.05$. The domain has $N = 40$ gridblocks, and the initial condition is expressed as: $S_{\text{lower}} = 0$ and $S_{\text{upper}} = 1$ (oil on the lower half of the domain and water above). The timestep size is 0.1 and the total simulation time is 2. The saturation distributions at the end of simulation appear in Fig. 2.13 where ‘God_4000’ indicates the Godunov flux with $N = 4000$, and could be viewed as a reference solution. From the results we can see that the three schemes Godunov, PPU and C1-PPU have almost the same level of dissipation for this simulation scenario, while the HU scheme is clearly more diffusive.

![Figure 2.13: Saturation distributions at the end of simulation for the viscous-dominated case](image)

Next, we present several test cases with $u_T = 0.01$, $M = 5$ and $C_g = 0.05$ to examine the impact of the nonlinearity and C1-continuity properties on the convergence performance.
Table 2.1: Nonlinear convergence performance for the cases with different initial conditions

<table>
<thead>
<tr>
<th>$S_{\text{init}}$ (lower)</th>
<th>$S_{\text{init}}$ (upper)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>C1-PPU</td>
<td>379</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>389</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>1252</td>
</tr>
<tr>
<td>0.2</td>
<td>0.2</td>
<td>C1-PPU</td>
<td>205</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>170</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>267</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>C1-PPU</td>
<td>1196</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>1193</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>1413</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>C1-PPU</td>
<td>379</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>389</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>1252</td>
</tr>
<tr>
<td>0.9</td>
<td>0.25</td>
<td>C1-PPU</td>
<td>81</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>283</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>98</td>
</tr>
</tbody>
</table>

The domain has $N = 1000$ gridblocks; the initial timestep size is 5 and the total simulation time is 30; the maximum allowable number of Newton iterations per timestep is set to 200. A heuristic damping strategy is employed to stabilize the Newton updates: the maximum absolute change in saturation remains as $\Delta S = 0.2$. The results for different initial conditions are shown in Table 6.1. The typical cases presented in the tables are selected to illustrate the impact of nonlinearity, which is deduced as the main reason for the performance degradation of the HU scheme. For most of the simulation cases we have conducted but not shown in the results, it is observed that our C1-PPU scheme is comparable to HU in the convergence rate. In addition, we can see that the performance of PPU is much worse, which clearly indicates the negative impact of the discontinuity in flux function.

We also run the buoyancy-dominated cases with $u_T = 0.01$, $M = 5$ and $C_g = 0.5$. The domain has $N = 500$ gridblocks. The results shown in Table 2.2 indicate that in addition to smoothness, nonlinearity is also critical for convergence behavior, and the C1-PPU scheme exhibits superior convergence rate compared to the other alternatives.
Table 2.2: Nonlinear convergence performance for the buoyancy-dominated cases

<table>
<thead>
<tr>
<th>S_{init} (lower)</th>
<th>S_{init} (upper)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.15</td>
<td>0.15</td>
<td>C1-PPU</td>
<td>438</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>1030</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>368</td>
</tr>
<tr>
<td>0.3</td>
<td>0.3</td>
<td>C1-PPU</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>1084</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>80</td>
</tr>
<tr>
<td>0.8</td>
<td>0.15</td>
<td>C1-PPU</td>
<td>517</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>1470</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>912</td>
</tr>
<tr>
<td>0.75</td>
<td>0.15</td>
<td>C1-PPU</td>
<td>221</td>
</tr>
<tr>
<td></td>
<td></td>
<td>HU</td>
<td>471</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PPU</td>
<td>335</td>
</tr>
</tbody>
</table>

2.6 Results: fully-coupled flow and transport

In the following simulation studies, convergence performance is not compared between the HU and C1-PPU schemes, because HU only applies to the fractional flow formulation with the separate equations for the parabolic and hyperbolic parts. The results illustrate that C1-PPU exhibits superior convergence rate for large time steps compared with PPU.

For the coupled flow and transport, an adaptive smoothing formula similar to Eq. (2.65) can be derived. Based on the generalized C1-PPU flux given by Eq. (2.87), the maximum error introduced by the smoothing function depends on the potential differences in the domain. We observe that a reasonable balance between the accuracy and convergence behavior can be achieved through the following formula for the smoothing coefficient $\epsilon$, which is related to the strength of the gravity force,

$$\epsilon = \kappa |\rho_\alpha g \Delta h|$$  \hspace{1cm} (2.124)

It is worth noting that for practical applications, a small variation in $\epsilon$ will not cause large impact on the solution performances. A reasonable balance between accuracy and nonlinear convergence can be achieved as long as the smoothing coefficient falls within the value range approximated by the adaptive formula.
2.6.1 Two-phase heterogeneous cases

2D heterogeneous cases are presented to evaluate the accuracy and convergence performance of the developed C1-PPU scheme. The basic specification of the synthetic model is shown in Table 5.1. Quadratic relative-permeability functions are used: $k_{rw} = S^2$ and $k_{ro} = (1 - S)^2$. The associated oil property data is shown in Table 4.2. The simulation control parameters are summarized in Table 2.5. A simple time-stepping strategy is employed in the simulator: if the Newton’s method fails to converge, time step is reduced by half until it converges; if a reduced time step is being used and the iteration number becomes less than the optimal number, the next time step will be doubled.

Table 2.3: Specification of the synthetic model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NX / NZ</td>
<td>100 / 100</td>
<td></td>
</tr>
<tr>
<td>LX / LY / LZ</td>
<td>30.48 / 0.3048 / 30.48</td>
<td>m</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2500</td>
<td>psi</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Initial Porosity</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>Rock compressibility</td>
<td>7E-4</td>
<td>1/psi</td>
</tr>
<tr>
<td>Rock reference pressure</td>
<td>2500</td>
<td>psi</td>
</tr>
<tr>
<td>Water reference pressure</td>
<td>3600</td>
<td>psi</td>
</tr>
<tr>
<td>Water reference viscosity</td>
<td>0.2</td>
<td>cP</td>
</tr>
<tr>
<td>Water compressibility</td>
<td>4E-6</td>
<td>1/psi</td>
</tr>
<tr>
<td>Water viscosibility Cvw</td>
<td>1.2E-6</td>
<td>1/psi</td>
</tr>
<tr>
<td>Water reference density</td>
<td>63.02</td>
<td>lb/ft3</td>
</tr>
<tr>
<td>Injection rate</td>
<td>0.1</td>
<td>m3/D</td>
</tr>
<tr>
<td>Production BHP</td>
<td>1000</td>
<td>psi</td>
</tr>
</tbody>
</table>

Table 2.4: Oil properties

<table>
<thead>
<tr>
<th>Pressure</th>
<th>Oil FVF</th>
<th>Oil viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>1.012</td>
<td>1.16</td>
</tr>
<tr>
<td>1200</td>
<td>1.004</td>
<td>1.164</td>
</tr>
<tr>
<td>2000</td>
<td>0.996</td>
<td>1.167</td>
</tr>
<tr>
<td>2800</td>
<td>0.988</td>
<td>1.172</td>
</tr>
<tr>
<td>3600</td>
<td>0.9802</td>
<td>1.177</td>
</tr>
<tr>
<td>4400</td>
<td>0.9724</td>
<td>1.181</td>
</tr>
<tr>
<td>5200</td>
<td>0.9646</td>
<td>1.185</td>
</tr>
<tr>
<td>5600</td>
<td>0.9607</td>
<td>1.19</td>
</tr>
</tbody>
</table>
Table 2.5: Simulation control parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step size</td>
<td>50</td>
<td>day</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>2000</td>
<td>day</td>
</tr>
<tr>
<td>Maximum number of nonlinear iterations</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Optimal number of nonlinear iterations</td>
<td>6</td>
<td></td>
</tr>
</tbody>
</table>

We consider two scenarios with different locations of producer and injector. The first scenario has an injector at the bottom left corner and a producer at the top right. Random Gaussian permeability field is generated in Fig. 2.14 and oil reference density is $10 \text{ lb/ft}^3$. In Fig. 2.15 we plot the oil saturation distributions at 100 day to examine the accuracy of the C1-PPU scheme. The results show that the dissipation level of C1-PPU is only slightly higher than PPU, and the difference between the two is almost negligible. In Table 2.6 we summarize the iteration number of the two schemes for different timestep sizes. The result of the case 'PPU (no gravity)' shows that computations are much faster without the gravity effect. This indicates that the counter-current flow can cause nonlinear convergence problem when PPU is used. Note that PPU is sensitive to small changes in the pressure distribution. In contrast, C1-PPU is less sensitive and thus leads to a better convergence performance.

![Random permeability field for the bottom injector case](image)

Figure 2.14: Random permeability field for the bottom injector case

The second scenario has the opposite well locations compared to the first scenario.
Figure 2.15: Oil saturation profiles for the bottom injector case at 100 day

Table 2.6: Iteration performance for the bottom injector case

<table>
<thead>
<tr>
<th>Time step size (day)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>C1-PPU</td>
<td>488</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>710</td>
</tr>
<tr>
<td>50</td>
<td>C1-PPU</td>
<td>230</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>403</td>
</tr>
<tr>
<td></td>
<td>PPU (no gravity)</td>
<td>178</td>
</tr>
</tbody>
</table>

The injector is placed at the top right corner. The random permeability field is plotted in Fig. 2.16. The oil saturation distributions at 100 day is shown in Fig. 2.17. The iteration number of the two schemes for different timestep sizes is summarized in Table 2.7. We also run a case with the oil reference density changed to 25 $lb/ft^3$, and the results are shown in Table 2.8. As can be seen, pronounced convergence difficulty is encountered with the PPU scheme for this case. This is because fluid flow in the domain is close to the state of gravity equilibrium, and the discontinuous switching behavior of PPU could easily cause severe restrictions on the timestep size. Compared with PPU, our C1-PPU scheme exhibits superior convergence performance and achieves reduction in the total Newton iterations by more than an order of magnitude.
Figure 2.16: Random permeability field for the top injector case

![Permeability Field](image)

Figure 2.17: Oil saturation profiles for the top injector case at 100 day

![Saturation Profiles](image)

Table 2.7: Iteration performance for the top injector case

<table>
<thead>
<tr>
<th>Time step size (day)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>C1-PPU</td>
<td>521</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>703</td>
</tr>
<tr>
<td>50</td>
<td>C1-PPU</td>
<td>295</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>525</td>
</tr>
</tbody>
</table>
Table 2.8: Iteration performance for the case with oil reference density reset to 25 lb/ft³

<table>
<thead>
<tr>
<th>Time step size (day)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>C1-PPU</td>
<td>228</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>6253</td>
</tr>
</tbody>
</table>

2.6.2 Two-phase flow in discrete fractured media

We run a two-phase flow case with two intersected fractures. The modified model parameters are summarized in Table 2.9. The other parameters specified in the examples from the last section remain unchanged. An injector is placed at the top left corner and a producer at the bottom right. The Cartesian model employ an explicit representation with logarithmic grid refinement for the discrete fractures.

Table 2.9: Specification of the synthetic model with discrete fractures

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>LX / LY / LZ</td>
<td>100 / 1 / 100</td>
<td>m</td>
</tr>
<tr>
<td>Fracture locations</td>
<td>(56, 20-80), (20-80, 56)</td>
<td></td>
</tr>
<tr>
<td>Fracture aperture</td>
<td>1E-03</td>
<td>m</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>1E-15</td>
<td>m²</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>1E-10</td>
<td>m²</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Oil reference density</td>
<td>10</td>
<td>lb/ft³</td>
</tr>
<tr>
<td>Injection rate</td>
<td>10</td>
<td>m³/D</td>
</tr>
<tr>
<td>Production BHP</td>
<td>2000</td>
<td>psi</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>500</td>
<td>day</td>
</tr>
</tbody>
</table>

To eliminate the impact of the temporal discretization error, we employ a small chopping limit $\Delta S = 0.05$ to generate the saturation profiles of the PPU scheme with stable time step. The oil saturation profiles at 500 day are shown in Fig. 2.18 and solution differences between the two schemes are minimal. We also run a second case with injection rate changed to $2 \ m^3/D$ and initial water saturation to 0.4. The iteration performance for different time step sizes is summarized in Tables 2.10 and 2.11. As we can see, for relatively large time steps, the C1-PPU scheme exhibits significantly better nonlinear performance compared to PPU, especially in the second simulation case.
It is interesting to note that even with a very small smoothing coefficient (e.g. $\epsilon = 1e^{-4}$), C1-PPU can still achieve a similar performance in the second case. This indicates that the non-differentiable PPU scheme is very sensitive to small amplitude noise near the switching region and thus greatly suffers from the local oscillations between iterations.

![Figure 2.18: Oil saturation profiles for the first case](image)

Table 2.10: Iteration performance for the first case

<table>
<thead>
<tr>
<th>Time step size (day)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>C1-PPU</td>
<td>1052</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>1094</td>
</tr>
<tr>
<td>5</td>
<td>C1-PPU</td>
<td>448</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>1311</td>
</tr>
<tr>
<td>10</td>
<td>C1-PPU</td>
<td>248</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>1289</td>
</tr>
</tbody>
</table>

2.6.3 Three-phase flow

We consider a compressible water-oil-gas system. We run two cases to examine accuracy and nonlinear convergence properties of the C1-PPU flux. The specification of the synthetic model is shown in Table 2.12. Aziz and Settari’s version of Stone’s model (Aziz and Settari, 1979) is used for the three-phase relative permeabilities. $S_{org}$, $S_{orw}$, $S_{gr}$ and $S_{wr}$
Table 2.11: Iteration performance for the second case

<table>
<thead>
<tr>
<th>Time step size (day)</th>
<th>Iterations</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>C1-PPU</td>
<td>1048</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>1118</td>
</tr>
<tr>
<td>5</td>
<td>C1-PPU</td>
<td>470</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>9203</td>
</tr>
<tr>
<td>10</td>
<td>C1-PPU</td>
<td>253</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>9712</td>
</tr>
</tbody>
</table>

are set to 0.1; \( e_{og}, e_g, e_{ow} \) and \( e_w \) are 1.0. The PVT properties for dry gas (PVDG) and dead oil (PVDO) are shown in Tables 2.14 and 4.2 respectively. The formation volume factor (FVF) is assumed to depend on the pressure only. The rock permeability shown in Fig. 2.19 represents the top layer of the SPE 10 model. There are one injector at the lower right corner and one producer at the middle of the reservoir. The simulation control parameters are summarized in Table 2.13.

Table 2.12: Specification of the three-phase synthetic model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NX / NZ</td>
<td>60 / 220</td>
<td></td>
</tr>
<tr>
<td>LX / LY / LZ</td>
<td>120 / 2 / 440</td>
<td>m</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2500</td>
<td>psi</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Initial porosity</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Oil reference density</td>
<td>45</td>
<td>lb/ft³</td>
</tr>
<tr>
<td>Water reference density</td>
<td>63</td>
<td>lb/ft³</td>
</tr>
<tr>
<td>Gas reference density</td>
<td>0.07</td>
<td>lb/ft³</td>
</tr>
<tr>
<td>Rock compressibility</td>
<td>1.0E-7</td>
<td>1/psi</td>
</tr>
<tr>
<td>Rock reference pressure</td>
<td>2500</td>
<td>psi</td>
</tr>
<tr>
<td>Water reference pressure</td>
<td>3600</td>
<td>psi</td>
</tr>
<tr>
<td>Water reference viscosity</td>
<td>0.2</td>
<td>cP</td>
</tr>
<tr>
<td>Water compressibility</td>
<td>4E-6</td>
<td>1/psi</td>
</tr>
<tr>
<td>Water viscosibility Cvw</td>
<td>1.2E-6</td>
<td>1/psi</td>
</tr>
<tr>
<td>Production BHP</td>
<td>1500</td>
<td>psi</td>
</tr>
</tbody>
</table>

The first case is a water flooding case, with 10 \( m^3/D \) injection rate. The initial gas saturation is 0.4. The second case describes a gas flooding process, and the injection rate is 40 \( m^3/D \). The initial gas saturation is changed to 0.2. The oil phase is chosen to compute the
Table 2.13: Simulation control parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial time step size</td>
<td>0.1</td>
<td>day</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>300</td>
<td>day</td>
</tr>
<tr>
<td>Maximum number of nonlinear iterations</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Optimal number of nonlinear iterations</td>
<td>7</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.14: PVDG

<table>
<thead>
<tr>
<th>Pressure (psi)</th>
<th>Gas FVF</th>
<th>Gas viscosity (cP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>9.683</td>
<td>0.013</td>
</tr>
<tr>
<td>900</td>
<td>3.108</td>
<td>0.019</td>
</tr>
<tr>
<td>1500</td>
<td>1.795</td>
<td>0.025</td>
</tr>
<tr>
<td>2100</td>
<td>1.252</td>
<td>0.031</td>
</tr>
<tr>
<td>3000</td>
<td>0.866</td>
<td>0.041</td>
</tr>
<tr>
<td>4000</td>
<td>0.7</td>
<td>0.05</td>
</tr>
<tr>
<td>5000</td>
<td>0.6</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Table 2.15: PVDO

<table>
<thead>
<tr>
<th>Pressure (psi)</th>
<th>Oil FVF</th>
<th>Oil viscosity (cP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>165</td>
<td>1.082</td>
<td>1.04</td>
</tr>
<tr>
<td>665</td>
<td>1.111</td>
<td>0.97</td>
</tr>
<tr>
<td>1165</td>
<td>1.146</td>
<td>0.9</td>
</tr>
<tr>
<td>1665</td>
<td>1.187</td>
<td>0.83</td>
</tr>
<tr>
<td>2502</td>
<td>1.263</td>
<td>0.72</td>
</tr>
<tr>
<td>4000</td>
<td>1.379</td>
<td>0.51</td>
</tr>
<tr>
<td>5000</td>
<td>1.45</td>
<td>0.39</td>
</tr>
</tbody>
</table>

Figure 2.19: Permeability field of the top layer in the SPE 10 model

smoothing coefficient $\epsilon$ through Eq. (2.124), resulting in $\epsilon = 2000$ for the C1-PPU scheme. The phase saturation profiles at the end of the simulations are shown in Figs. 2.20 2.21 2.22 and 2.23. We can see that the C1-PPU scheme is a little more diffusive than PPU, but within an acceptable level of the overall solution accuracy.
Linear system is solved by the ILU0-GMRES iterative solver. Table 2.16 summarizes the iteration number and CPU time ratio of the two schemes. Compared to the PPU scheme, C1-PPU leads to much larger time step advancement and faster nonlinear convergence. PPU produces oscillations in the Newton updates, and subsequently suffer from serious convergence problems. For the two cases, a reduction of nearly 60% in the computational cost is obtained.

Figure 2.20: Oil saturation profiles for the water injection case
Figure 2.21: Water saturation profiles for the water injection case

Table 2.16: Computational performance for the three-phase cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Iterations</th>
<th>CPU time ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water injection</td>
<td>C1</td>
<td>1183</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>1926</td>
</tr>
<tr>
<td>Gas injection</td>
<td>C1</td>
<td>225</td>
</tr>
<tr>
<td></td>
<td>PPU</td>
<td>359</td>
</tr>
</tbody>
</table>
Figure 2.22: Gas saturation profiles for the gas injection case
Figure 2.23: Oil saturation profiles for the gas injection case
3.1 Mimetic finite difference method for phase velocities

Accurate representation of complex reservoir geology using unstructured meshes, and upscaling of high-resolution geostatistical reservoir model into full-tensor permeability fields would pose big challenges for numerical discretization techniques in reservoir simulation (Alpak 2010). Combined effects of grid non-orthogonality induced by mesh distortion and strong permeability anisotropy cannot be resolved by conventional two-point flux approximation scheme (TPFA). These factors may lead to large errors in flow predictions (Edwards and Rogers 1998; Aavatsmark 2002). Several consistent discretization schemes such as the multi-point flux approximation (MPFA), mixed finite-element (MFE) and mimetic finite difference (MFD) methods were developed to overcome these challenges. Here we focus on the MFD method to approximate the phase velocities in Equation \((2.3)\). MFD exhibits some advantageous characteristics: 1) locally conservative, 2) second-order accurate for cell-center potential and first-order accurate for cell-face flux on smoothly distorted meshes with heterogeneous and fully anisotropic permeability field and 3) leads to a sparse symmetric positive definite coefficient matrix (Alpak 2010).

For simplicity, let us consider the incompressible single-phase flow equation,

\[ \nabla \cdot \mathbf{u} = q , \quad \mathbf{u} = -K \nabla p \quad (3.1) \]

A consistent, finite-volume formulation for general polygonal and polyhedral meshes gives
the cell-based, local discretization as (Lie et al. 2012),

$$\mathbf{u}_i = \mathbf{T}_i (\mathbf{e} p_i - \pi_i) \quad (3.2)$$

where now the phase dependency has been removed and $\mathbf{u}_i$ is a vector of all fluxes associated with a cell $\Omega_i$; $\mathbf{e} = (1,\ldots,1)^T$; $\pi_i$ is a vector of face pressures, and $\mathbf{T}_i$ is a matrix of one-sided transmissibilities. The local discretization could also be written as,

$$\mathbf{M}_i \mathbf{u}_i = \mathbf{e} p_i - \pi_i \quad (3.3)$$

where the matrix $\mathbf{M}_i$ is referred to as the local inner product.

In the following formulation, the continuity of fluxes across cell faces is introduced as a set of equations that together with mass conservation and Darcy’s law constitute a coupled system for cell pressure, face pressure, and fluxes. By collecting the local discretization on each cell, we could derive a linear system of discrete global equations (Singh 2010):

$$\begin{bmatrix} \mathbf{M} & \mathbf{E} & \mathbf{L} \\ \mathbf{E}^T & 0 & 0 \\ \mathbf{L}^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ -\mathbf{p} \\ \pi \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{Q} \\ 0 \end{bmatrix} \quad (3.4)$$

where the first row in the block-matrix equation corresponds to Equation (3.3) for all grid cells. The vector $\mathbf{u}$ contains the outward fluxes associated with half faces ordered cell-wise, the vector $\mathbf{p}$ contains the cell pressures, and $\pi$ the face pressures. The matrices $\mathbf{M}$ and $\mathbf{E}$ are block diagonal with each block corresponding to a cell. Each column of $\mathbf{L}$ corresponds to a unique interface in the grid and has two unit entries for interfaces between cells in the interior of the grid. Similarly, $\mathbf{L}$ has a single unit entry in each column that corresponds to an exterior interface.

MFD methods are constructed so that they are exact for linear pressure fields and give a symmetric positive-definite matrix $\mathbf{M}_i$. Consider two neighboring gridcells $i$ and $j$
with interface \( E \), shown in Figure 3.1. Let \( n_{ij} \) denote the area-weighted normal vector to \( E \) and \( x_{ij} \) be the vector pointing from the centroid of cell \( \Omega_i \) to the centroid of face \( E \). All vectors \( x_{ij} \) and \( n_{ij} \) defined for the cell \( \Omega_i \) are collected as rows in two matrices \( X_i \) and \( N_i \). It has been shown that the matrices \( M_i \) and \( T_i \) must satisfy the following consistency conditions (Brezzi et al. 2005),

\[
\begin{align*}
MNK &= X, \quad \text{and} \quad NK = TX
\end{align*}
\]

(3.5)

How to obtain a symmetric positive-definite matrix \( M_i \) is the key step for the MFD method. A strict theorem is presented by Brezzi et al. (2005), where they give a recipe for constructing \( M_i \). The symmetric and positive definite inner product that fulfills Equation (3.5) can be represented in the compact form,

\[
M = \frac{1}{|\Omega_i|} X K^{-1} X^T + Q_N^\perp S_M Q_N^\perp^T
\]

(3.6)

\[
= \frac{1}{|\Omega_i|} X K^{-1} X^T + P_N^\perp S_M P_N^\perp^T
\]

where \( S_M \) denotes any symmetric, positive definite matrix, \( Q_N^\perp \) is an orthonormal basis for the left null space of \( N^T \), and \( P_N^\perp \) is the null-space projection \( I - Q_N Q_N^T \) in which \( Q_N \) is a basis for the spaces spanned by the columns of \( N \).

Similarly, we can derive a closed expression for the inverse inner product \( T \),

\[
T = \frac{1}{|\Omega_i|} N K N^T + Q_X^\perp S_T Q_X^\perp^T
\]

(3.7)

\[
= \frac{1}{|\Omega_i|} N K N^T + P_X^\perp S_T P_X^\perp
\]

where \( Q_X^\perp \) is an orthonormal basis for the left nullspace of \( X^T \) and \( P_X^\perp = I - Q_X Q_X^T \) is the corresponding nullspace projection.

In this work, the following inverse inner product has been used (Singh 2010),

\[
T = \frac{1}{|\Omega_i|} \left[ N K N^T + \frac{6}{d} \text{trace}(K) A (I - Q Q^T) A \right]
\]

(3.8)
where $A$ is the diagonal matrix containing face areas and $Q = \text{orth}(AX)$; $d$ the space dimension; and $I$ the identity matrix.

![Geometric ingredients for the connection between two neighboring gridcells](image)

Figure 3.1: Geometric ingredients for the connection between two neighboring gridcells

It should be noted that the contribution of the gravity force is not incorporated in Equation (3.2) for the calculation of face fluxes. Here we intend to directly work with the coupled mass conservation equations instead of the popular fractional flow formulation. Recall that in the MFD method the flux continuity is ensured through a set of constraint equations that equate the fluxes from the two adjacent cells of an interface. We observe that the continuities of the both phase fluxes can be simultaneously attained only if a single value is used for the gravity part. Therefore the scalar quantities for $K \nabla h$ are first computed from the properties of the two adjacent cells using similar formulae as Equation (3.2). Then the arithmetic average of the scalar quantities are used to compute the gravity flux $G_i$. The discrete phase fluxes now can be expressed as,

$$F_{\alpha i} = \rho_{\alpha} \frac{k_{\alpha}}{\mu_{\alpha}} (u_i + G_i)$$  \hspace{1cm} (3.9)

### 3.2 Fully-implicit high-resolution CCFV framework

First-order schemes include large numerical diffusion effect and thus give a poor solution. A higher-order scheme provides a better resolution and reduces the smoothing near
shocks. In the field of flow through porous media, explicit temporal schemes are usually considered impractical due to large variations in the Darcy velocity and porosity field. Therefore, implicit schemes capable of taking larger time steps are preferred in practical computations. However, even for a simple first-order method, solving a large nonlinear system is often very expensive; Extra coupling and nonlinearity of the discretised equations can be introduced from a higher-order discretisation (Natvig and Lie 2008). It has been shown that strong nonlinearity as well as lack of continuous differentiability in the numerical flux function and flux limiter can cause serious nonlinear convergence problems.

In this work we intend to develop a fully-implicit CCFV framework that could achieve second-order spatial accuracy on smooth solutions, while at the same time maintain robustness and nonlinear convergence performance. We target two essential components of a high-resolution FV scheme: the variable reconstruction and the flux limiter. We develop a novel multislope MUSCL method and an adaptive limiting strategy that have improved computational efficiency, smoothness properties, and accuracy. The reconstruction scheme interpolates the required values at the edge centroids in a simple way by taking advantage of some geometric features of the triangular mesh. The numerical diffusion induced by mesh skewness is reduced, and optimal second order accuracy can be achieved without sacrificing robustness. An improved smooth piecewise-linear flux limiter is introduced to provide high accuracy without degrading nonlinear convergence behavior on non-uniform mesh.

The Phase-Potential Upwinding (PPU) scheme is employed to compute the numerical flux which depends on the two reconstructed saturation states at the cell edge. In PPU, the upstream direction of a fluid phase is determined according to the gradient of its potential across the interface between two cells.

3.3 Multislope MUSCL schemes

Traditional high-order schemes often produce spurious oscillations at discontinuities due to their unbounded behavior. Equipping the high-order schemes with the boundedness property leads to the so-called high-resolution schemes (HRS), which are able to provide
good resolution near steep gradients without introducing spurious oscillations (Zhang et al. 2015). In HRS, high-order schemes can be combined with flux limiters to maintain the TVD property. The flux limiters use a measure of local monotonicity to switch between a first-order and high-order scheme (Denner and van Wachem 2015).

On the one hand, there exists a large family of MUSCL techniques: a unique gradient is first computed for each cell element through the neighbouring values. Then the gradient is modified to obey some Maximum Principle or TVD constraint and provide a vectorial slope on the element (Calgaro et al. 2010). New values are subsequently reconstructed on element edges. Finally, the two computed values on both sides of the edge are used to approximate the numerical flux. The MUSCL method presented above is referred to as monoslope (or cell-based) method since the reconstructed values are obtained using the same vectorial slope on each element (Buffard and Clain 2010).

In contrast to these methods, a class of multislope methods have been recently developed in the literature to deal with MUSCL reconstructions on unstructured meshes (Calgaro et al. 2010; Clain et al. 2010; Hou et al. 2014; Le Touze et al. 2015). A specific scalar slope for each interface is computed to represent an approximation of the directional derivatives (Clain et al. 2010). The slopes are subsequently modified through an efficient edge-based limiting procedure that can avoid the additional loop required for cell-based limiting methods to select the best limiter among faces and greatly reduce the number of times the limiter is invoked (Hou et al. 2014). The multislope method also appears to be more robust and able to attain better accuracy than its monoslope counterpart (Le Touze et al. 2015). Moreover, as was pointed out by Delis and Nikolos (2013), the face-based limiters chatter far less than the cell-based ones and thus can achieve better iterative convergence performance. Note that the multislope reconstruction does not provide any piecewise function whereas the monoslope technique gives a linear function on each cell which satisfies the conservative property. However, the shape of the reconstructed function inside the cell is not of importance for finite volume method, where only flux evaluations at the edges of cell are essential (Buffard and Clain 2010).
3.3.1 Review of the existing multislope schemes

Here we review a recently proposed multislope MUSCL scheme (Buffard and Clain 2010) for the reconstruction of saturation variables. To demonstrate the numerical discretization, we introduce the following geometric ingredients shown in Figure 3.2. The domain consists of triangles $\Omega_i$ with centroid $B_i$. For a given $i$, $v(i)$ represents the index set of the common edge elements $\Omega_j$, $j \in v(i)$ where $E_{ij}$ stands for the common edge. Point $Q_{ij}$ is defined as the intersection between the segment $B_iB_j$ and the line $E_{ij}$.

![Figure 3.2: Geometric ingredients and notations](image)

In order to obtain second-order spatial accuracy, the saturation variables at the left and right sides of the edge ($S_L$ and $S_R$, respectively) are reconstructed to compute the numerical fluxes $F_{ij}(S_L, S_R)$ using the Godunov-type finite volume scheme (Le Touze et al. 2015). To build the multislope method, we first introduce the barycentric coordinates $\lambda_k$,

$$\sum_{k=1,2,3} \lambda_k B_{jk} = B_i, \quad \sum_{k=1,2,3} \lambda_k = 1 \quad (3.10)$$

It is assumed that the Delaunay mesh satisfies the following hypothesis: the $B_i$ point is strictly inside the triangle formed by the three other points $B_{jk}$. Therefore $\lambda_k > 0$. Defining a set of normalized vectors,

$$t_k = t_{ijk} = \frac{B_iB_{jk}}{|B_iB_{jk}|}, \quad k = 1, 2, 3 \quad (3.11)$$
Using Equation (3.10), we obtain a decomposition (referred to as the fundamental decomposition) of \( t_k \) as a function of the two other directions,

\[
\begin{align*}
  t_1 &= \beta_{12} t_2 + \beta_{13} t_3, \\
  t_2 &= \beta_{21} t_1 + \beta_{23} t_3, \\
  t_3 &= \beta_{31} t_1 + \beta_{32} t_2.
\end{align*}
\]

(3.12)

with \( \beta_m \beta_l = 1 \) and \( \beta_m \beta_l = -\beta_m \), for any circular permutation \((m, l, k)\) of \((1, 2, 3)\) and all the coefficients are negative. Then two sets of slopes are constructed. We define the downstream slopes with respect to point \( B_i \) in direction \( t_{ij} \) by,

\[
(\nabla S)_{ijk}^+ = \frac{S_{jk} - S_i}{|B_iB_j|}, \quad k = 1, 2, 3
\]

(3.13)

and we define the upstream slopes as,

\[
\begin{align*}
(\nabla S)_{ij1}^- &= \beta_{12} (\nabla S)_{ij2}^+ + \beta_{13} (\nabla S)_{ij3}^+, \\
(\nabla S)_{ij2}^- &= \beta_{21} (\nabla S)_{ij1}^+ + \beta_{23} (\nabla S)_{ij3}^+, \\
(\nabla S)_{ij3}^- &= \beta_{31} (\nabla S)_{ij1}^+ + \beta_{32} (\nabla S)_{ij2}^+.
\end{align*}
\]

(3.14)

Now we give a definition of the flux limiter \( \psi (a, b) \) to provide the stability property for the reconstruction. For example, Van Leer’s limiter,

\[
\psi (a, b) = \frac{ab + |ab|}{a + b + e}
\]

(3.15)

where \( e = 10^{-12} \) is used to prevent division by zero. The limited slopes in the \( t_{ij} \) direction are defined by,

\[
(\nabla S)_{ij} = \psi ((\nabla S)_{ij}^+, (\nabla S)_{ij}^-)
\]

(3.16)
Finally, $S_L$ can be evaluated in the one-dimensional form,

$$S_L = S_i + (\nabla S)_{ij} |B_iQ_{ij}|, \quad j \in v(i)$$

(3.17)

It should be noted that there also exists a large number of works in the literature that focus on the so-called r-ratio formulations for TVD schemes (Delis and Nikolos 2013; Kong et al. 2013; Hou et al. 2013; Denner and van Wachem 2015; Zhang et al. 2016). We notice that the previously mentioned multislope concept that is based on a "face by face" limiting process essentially coincides with the r-ratio schemes. In this class of schemes, the r-ratio is employed as a measure of local monotonicity through the flux limiters. Although the implementation of r-ratio schemes on equidistant Cartesian meshes in a multidimensional context is straightforward, the implementation of such schemes on unstructured meshes is more difficult due to geometric complexity and mesh skewness. The most frequently cited problem is the determination of a far-upwind node that is necessary for a TVD formulation, which is not readily available on unstructured meshes (Denner and van Wachem 2015). For example in Figure 3.3 if flow is from center cell C towards the downstream cell D, point U denotes the virtual far-upwind node. Using the r-ratio formulation with flux limiter for non-uniform meshes, $S_L$ can be rewritten as,

$$S_L = S_C + \frac{|CQ|}{|UC|} \psi(r) (S_C - S_U)$$

(3.18)
where,

$$r = \left( \frac{S_D - S_C}{|CD|} \right) / \left( \frac{S_C - S_U}{|UC|} \right)$$  \hspace{1cm} (3.19)$$

It can be verified that the multislope MUSCL reconstruction shown in Equation (3.17) is essentially identical to the formulae of Equation (3.18). We can see that the intersection point $H_{ij}$ in Figure 3.2 becomes the virtual far-upwind node, and its value is computed through the inverse distance-weighted interpolation of the cell values at $B_{j2}$ and $B_{j3}$.

The multislope MUSCL method reviewed in the last section reconstructs the saturation variables at the point $Q$ (the intersection point of the considered edge and the line passing through the two adjacent cell centroids, see Figure 3.3), which does not generally coincide with the midpoint $M$ of the edge where fluxes are evaluated. This issue is commonly referred to as mesh skewness and can introduce a large diffusion-like error in the solution on poorly connected grids (Denner and van Wachem 2015). The numerical flux $F_{ij}$ is an approximation of the exact flux integrated on edge $E$. Numerical integration using edge midpoint for the quadrature formula provides a second-order approximation (Delis and Nikolos 2013). Therefore, better accuracy shall be obtained using $M$ in place of $Q$ (Hou et al. 2013). Several correction strategies were proposed to compute the reconstructed values at $M$ (Buffard and Clain 2010; Hou et al. 2013; Delis and Nikolos 2013; Denner and van Wachem 2015). Although these methods can avoid the order reduction caused by mesh skewness, additional complexity and computation is involved due to the two-step correction procedure, where the value at $Q$ has to be evaluated first (Hou et al. 2013). Therefore, a straightforward edge-based MUSCL scheme that can directly reconstruct the midpoint values is highly desirable.

For a high-resolution scheme to be free of spurious oscillation, the reconstruction has to respect a local maximum principle, and thus possess the $L^\infty$ stability. Le Touze et al. (2015) shows that such a scheme should satisfy the following sufficient condition for a CFL-independent limiter,

$$0 \leq \psi(r) \leq \min (\eta^+, \eta^- r)$$  \hspace{1cm} (3.20)$$

where the geometric parameters associated with the upstream and downstream slopes are
defined as,
\[ \eta^- = \frac{|UC|}{|CQ|}, \quad \eta^+ = \frac{|CD|}{|CQ|} \]  
(3.21)

For a uniform structured mesh, the geometric parameters can be simply replaced with the constants,
\[ 0 \leq \psi(r) \leq \min (2, 2r) \]  
(3.22)

In order to preserve the stability condition in Equation (3.20), modified flux limiters need to be designed according to the mesh irregularity and non-uniformity. However, as can be easily seen in Figure 3.2, the presented multislope scheme may lead to large variations in the parameters \( \eta^- \) and \( \eta^+ \) on highly distorted meshes. Thus it is very challenging to develop an adaptive limiting strategy to strictly ensure the stability, while still achieve high accuracy. Note that the violation of the monotonicity property could easily cause severe degradation in the nonlinear convergence performance of a fully-implicit scheme.

Several r-ratio schemes implicitly determine the virtual far-upwind node by extrapolation using the gradient of the considered cell (Darwish and Moukalled 2003; Hou et al. 2013; Delis and Nikolos 2013). The gradient can be constructed from the values of the neighboring cells. Kong et al. (2013) argues that this kind of scheme may generate non-physical overshoots and undershoots in the solution variables. The r-ratio scheme that determines the virtual far-upwind value by interpolation rather than extrapolation can avoid this problem and give more accurate predictions because more upwind information is included (Kong et al. 2013; Hou et al. 2013; Zhang et al. 2016).

3.3.2 A novel multislope scheme

In this work a novel multislope method is devised to directly construct the required values at the edge midpoint and strictly comply with the stability condition. This ensures that the method is able to reach an optimal second-order accuracy on smooth solutions with no sacrifice of robustness issues. The geometric notations are shown in Figure 3.4. The scheme is constructed by utilizing some useful geometrical invariant features of the triangular
grids. We notice that a line extending from a cell-vertex through the cell-centroid will always intersect the midpoint of the opposing edge. Moreover, in 2D the distance from the cell-vertex to the cell-centroid is always two-thirds of that from the vertex to the opposing edge. This geometric property is very favorable because the corresponding ratio \( \eta \) is identical with the constant obtained from uniform structured mesh. In this way, an optimal virtual far-upwind node is obtained at the cell-vertex \( U_{ij} \). Since the cell-centered method is employed, we need to first coalesce surrounding cell information to the vertices of the candidate cell. The vertex values are obtained by summing the values of neighboring cells with the weighting of inversely proportional distance from vertex to centroid (Park et al. 2010),

\[
S_{v_i} = \frac{\sum_k (S_k/r_{v_i,k})}{\sum_k r_{v_i,k}^{-1}} \tag{3.23}
\]

where \( S_{v_i} \) is the value at the vertex \( v_i \), and \( r_{v_i,k} \) is the distance from \( v_i \) to the neighboring cell \( \Omega_k \). The notations for the computation of the vertex value are shown in Figure 3.5.

The evaluation of the downstream slope is also straightforward and only needs the solution variables that are readily available. We define the intersection point \( H_{ij} \) between the line \((B_iH_{ij})\) and the segment \((B_jV_{ij})\). \( V_{ij} \) is a vertex of the downstream cell \( B_j \), and can be easily determined according to the position of \( M_{ij} \) relative to \( Q_{ij} \). Then the value at
Figure 3.5: Notations for the computation of the vertex value

\( H_{ij} \) is computed through a simple weighted means,

\[
S_{H_{ij}} = \beta_{ijv}S_{V_{ij}} + \beta_{ijb}S_{B_{ij}}
\]  

(3.24)

where,

\[
\beta_{ijv} = \frac{|B_{ij}H_{ij}|}{|B_{ij}V_{ij}|} \geq 0, \quad \beta_{ijb} = \frac{|V_{ij}H_{ij}|}{|B_{ij}V_{ij}|} \geq 0, \quad \beta_{ijv} + \beta_{ijb} = 1
\]  

(3.25)

Now the upstream and downstream slopes are computed as,

\[
(\nabla S)^- = \frac{S_i - S_{vi}}{|B_{ij}U_{ij}|}, \quad (\nabla S)^+ = \frac{S_{H_{ij}} - S_i}{|B_{ij}H_{ij}|}
\]  

(3.26)

The saturations at the edge are reconstructed using Equation (3.18).

It should be noted that the developed multislope method only applies to triangular/tetrahedral grids. Here we focus on this type of unstructured grids because it is the most popular and robust grid for meshing a discrete fractured media. Compared to the reviewed Buffard and Clain’s method, the novel method does not suffer from the mesh geometric constraint (i.e. \( \lambda_k > 0 \)), and thus can be safely employed on highly non-uniform and distorted meshes. The novel method also provides a simple and efficient way to obtain the required values at the edge midpoint. Moreover, higher accuracy should be achieved through the genuine upwind treatment and the optimal determination of far-upwind node.
3.4 $L^\infty$ stability of the novel multislope scheme

We show in this section that the finite-volume discretization equipped with the novel multislope scheme can be written as a positive scheme with bounded coefficients, thereby implying a Discrete Maximum Principle (DMP) and subsequently the $L^\infty$ stability,

**Definition 3.4.1 (DMP).** The MUSCL scheme complies with the DMP if for any element $\Omega_i$, the updated value at time $t^{n+1}$ is bounded by the minimum and maximum values at time $t^n$ within $\Omega_i$ and a given neighborhood $U(\Omega_i)$, which can be *a priori* of arbitrary extent. Let $\overline{U}_i$ denote the union $U(\Omega_i) \cup \{\Omega_i\}$, then the DMP formally reads in,

$$\min_{\Omega_j \in \overline{U}_i} S^n_j \leq S^{n+1}_i \leq \max_{\Omega_j \in \overline{U}_i} S^n_j$$

(3.27)

We follow a similar procedure as presented in Clain and Clauzon (2010) and Le Touze et al. (2015) to complete the proof. For simplicity, we consider a scalar hyperbolic conservation equation. The discretization of the domain consists of triangles $\Omega_i$. For a given $i$, $v(i)$ represents the index set of the common edge elements $\Omega_j$, $j \in v(i)$ where $E_{ij} = \Omega_i \cap \Omega_j$ stands for the common edge. In addition to $v(i)$, we now define the $w(i)$ neighborhood as the set of elements sharing at least a vertex with $\Omega_i$. Note that $v(i) \subset w(i)$. Let $(t^n)_{n \in [0,N]}$ be a discretization of time, and $\Delta t = t^{n+1} - t^n$ be the time step. The cell-centered finite-volume formulation with first-order accuracy reads in,

$$S^{n+1}_i = S^n_i - \Delta t \sum_{j \in v(i)} \frac{|E_{ij}|}{|\Omega_i|} F_{ij}(S_i, S_j, n_{ij})$$

(3.28)

where $F_{ij}(S_i, S_j, n_{ij})$ is the numerical flux function. For second-order MUSCL strategy, new arguments are provided to the numerical flux, without modification of the finite-volume scheme. The cell-centered states $S_i$ and $S_j$ are replaced respectively by interpolated states $S_{ij}$ and $S_{ji}$ on the edges $E_{ij}$. We now drop the dependency of the numerical flux on the
normal vector \( \mathbf{n}_{ij} \) for the sake of simplicity. The MUSCL scheme then reads in,

\[
S_i^{n+1} = S_i^n - \Delta t \sum_{j \in v(i)} \frac{|E_{ij}|}{|\Omega_i|} F_{ij}(S_{ij}, S_{ji}) \quad (3.29)
\]

As in the novel multislope scheme, both a backward and forward scalar slopes, respectively written \((\nabla S)^-_ij\) and \((\nabla S)^+_ij\), are computed for each edge \(E_{ij}\) of a given element \(\Omega_i\). The reconstructed values read as follows,

\[
S_{ij} = S_i + (\nabla S)^+_ij \psi(r_{ij}) |\mathbf{B}_i \mathbf{M}_{ij}| \\
S_{ji} = S_j + (\nabla S)^+_ji \psi(r_{ji}) |\mathbf{B}_j \mathbf{M}_{ij}| \quad (3.30)
\]

where \(\psi(r_{ij})\) is a limiter function and \(r_{ij} = (\nabla S)^-_ij/(\nabla S)^+_ij\).

### 3.4.1 Properties of the numerical flux and first rewriting of the scheme

The numerical flux \(F_{ij}\) at a given edge is a function of two variables, denoted for instance \(S_1\) and \(S_2\),

\[
F_{ij} = F_{ij}(S_1, S_2) \quad (3.31)
\]

where \(S_1\) and \(S_2\) are both assigned a certain evaluation of the scalar function coming from each side of \(E_{ij}\). Let us afterwards lay down some classical necessary properties of the numerical flux. Firstly, it has to be consistent with the physical flux \(\mathbf{F}\). If we assume a case where the scalar field has any uniform value \(S\), then the condition of consistency of the numerical flux reads in,

\[
F_{ij}(S, S) = \mathbf{F}(S) \cdot \mathbf{n}_{ij} \quad (3.32)
\]

which implies the useful relation,

\[
\sum_{j \in v(i)} |E_{ij}| F_{ij}(S, S) = \mathbf{F}(S) \cdot \sum_{j \in v(i)} |E_{ij}| \mathbf{n}_{ij} = 0 \quad (3.33)
\]
Secondly, the numerical flux has to be monotonous,

\[
\frac{\partial F_{ij}(S_1, S_2)}{\partial S_1} \geq 0, \quad \frac{\partial F_{ij}(S_1, S_2)}{\partial S_2} \leq 0
\]  

(3.34)

According to relation (3.33), we can rewrite the scheme (3.29) as,

\[ S_i^{n+1} = S_i^n - \sum_{j \in v(i)} \Delta t \frac{|E_{ij}|}{|\Omega_i|} \left( F_{ij}(S_{ij}, S_{ji}) - F_{ij}(S_{ij}, S_i) + F_{ij}(S_{ij}, S_i) - F_{ij}(S_i, S_i) \right) \]  

(3.35)

The mean value theorem provides the following relations:

\[ \exists S_{ij} \in \left( \min(S_i, S_{ij}), \max(S_i, S_{ij}) \right), \exists S_{ij}^* \in \left( \min(S_i, S_{ji}), \max(S_i, S_{ji}) \right), \]

such that,

\[
\frac{\partial F_{ij}}{\partial S_1}(S_{ij}^*, S_i) = \frac{F_{ij}(S_{ij}, S_i) - F_{ij}(S_i, S_i)}{S_{ij} - S_i}
\]  

(3.36)

\[
\frac{\partial F_{ij}}{\partial S_2}(S_{ij}, S_{ij}^*) = \frac{F_{ij}(S_{ij}, S_{ji}) - F_{ij}(S_{ij}, S_i)}{S_{ji} - S_i}
\]  

(3.37)

which leads to,

\[ S_i^{n+1} = S_i^n - \sum_{j \in v(i)} \Delta t \frac{|E_{ij}|}{|\Omega_i|} \left( \frac{\partial F_{ij}}{\partial S_1}(S_{ij}^*, S_i)(S_{ij} - S_i) + \frac{\partial F_{ij}}{\partial S_2}(S_{ij}, S_{ij}^*)(S_{ji} - S_i) \right) \]  

(3.38)

Next, we introduce the parameters below, which are nonnegative due to the monotonicity of the numerical flux,

\[ v_{ij}^+ = \Delta t \frac{|E_{ij}|}{|\Omega_i|} \frac{\partial F_{ij}}{\partial S_1}(S_{ij}^*, S_i) \geq 0, \quad v_{ij}^- = -\Delta t \frac{|E_{ij}|}{|\Omega_i|} \frac{\partial F_{ij}}{\partial S_2}(S_{ij}, S_{ij}^*) \geq 0 \]  

(3.39)

So we finally have the scheme under the form,

\[ S_i^{n+1} = S_i^n + \sum_{j \in v(i)} \left( v_{ij}^-(S_{ji} - S_i) - v_{ij}^+(S_{ij} - S_i) \right) \]  

(3.40)

From this point forward, the objective is to rewrite the differences \( S_{ij} - S_i \) and \( S_{ji} - S_i \) so
that we can write the scheme under the form,

\[ S_{i}^{n+1} = S_{i}^{n} + \sum_{j \in w(i)} c_{ij} (S_{j} - S_{i}), \quad \text{with} \quad c_{ij} \geq 0 \quad \text{and} \quad \sum_{j \in w(i)} c_{ij} \leq 1 \quad (3.41) \]

Note that we expect a sum on the \( w(i) \) neighborhood instead of the \( v(i) \) neighborhood, since the reconstruction procedure involves elements belonging to \( w(i) \).

### 3.4.2 Focus on the term \( S_{ij} - S_{i} \)

As explained in Clain and Clauzon (2010), the classical strategy to get a nonnegative coefficient for this term consists in achieving an inversion sign property as follows,

\[ S_{ij} - S_{i} = \sum_{k \in w(i)} \omega_{ijk} (S_{i} - S_{k}), \quad \omega_{ijk} \geq 0 \quad \text{and} \quad \sum_{k \in w(i)} \omega_{ijk} \leq C_{\infty} \quad (3.42) \]

where \( j \in v(i) \) and \( k \in w(i) \). \( C_{\infty} \) is a uniform constant. To do so, let us rewrite this term using the different relations given in the previous sections. We first introduce the geometric parameters,

\[ \eta_{ij}^- = \frac{|B_{ij}U_{ij}|}{|B_{ij}M_{ij}|}, \quad \eta_{ij}^+ = \frac{|B_{ij}H_{ij}|}{|B_{ij}M_{ij}|} \quad (3.43) \]

Using Equations (3.26) and (3.30), it comes,

\[ S_{ij} - S_{i} = |B_{ij}M_{ij}| (\nabla S)_{ij}^{+} \psi_{ij} = |B_{ij}M_{ij}| \frac{\nabla S_{ij}^{+}}{r_{ij}} \psi_{ij} = \frac{\psi_{ij}}{\eta_{ij}^- r_{ij}} (S_{i} - S_{v_{i}}) \quad (3.44) \]

According to Equation (3.23), we can write,

\[ S_{vi} = \sum_{l} \beta_{ij_{l}}^{-} S_{ij_{l}}^{-}, \quad \sum_{l} \beta_{ij_{l}}^{-} = 1 \quad (3.45) \]

where \( S_{ij_{l}}^{-} \) is the value in the cell \( \Omega_{ij_{l}}^{+} \) which belongs to \( w(i) \). Therefore,

\[ S_{ij} - S_{i} = \frac{\psi_{ij}}{\eta_{ij}^- r_{ij}} \left( S_{i} \sum_{l} \beta_{ij_{l}}^{-} - \sum_{l} \beta_{ij_{l}}^{-} S_{ij_{l}}^{-} \right) = \frac{\psi_{ij}}{\eta_{ij}^- r_{ij}} \sum_{l} \beta_{ij_{l}}^{-} (S_{i} - S_{ij_{l}}^{-}) \quad (3.46) \]
Finally, if we introduce the notation,

\[ L_{ij}^- = \{ \Omega_{ij}^- \mid l \in \mathbb{N} \} \]  

(3.47)

To denote the set of backward neighboring elements, then we come up with,

\[ S_{ij} - S_i = \sum_{k \in w(i)} \omega_{ijk} (S_i - S_k) \]  

(3.48)

with \( \omega_{ijk} = \frac{\psi_{ij}}{\eta_{ij} r_{ij}} \beta_{ij}^- \) if \( \Omega_k \in L_{ij}^- \), and \( \omega_{ijk} = 0 \) if \( \Omega_k \notin L_{ij}^- \). So we do have the nonnegativity of the \( \omega_{ijk} \) if the limiter is such that \( \psi_{ij} = 0 \) for \( r_{ij} \leq 0 \), and \( \psi_{ij} \geq 0 \) when \( r_{ij} > 0 \). Besides, the sum reads in,

\[ \sum_{k \in w(i)} \omega_{ijk} = \frac{\psi_{ij}}{\eta_{ij} r_{ij}} \]  

(3.49)

which will be uniformly bounded with an ad hoc limiter.

3.4.3 Focus on the term \( S_{ji} - S_i \)

According to relation (3.30), we have,

\[ S_{ji} - S_i = S_j - S_i + \frac{|B_j M_{ij}|}{|B_j H_{ji}|} \psi_{ji} (S_{H_{ji}} - S_j) \]  

(3.50)

\[ S_{ji} - S_i = (S_j - S_i) \left( 1 - \frac{\psi_{ji}}{\eta_{ji}} \right) + (S_{H_{ji}} - S_i) \frac{\psi_{ji}}{\eta_{ji}} \]  

(3.51)

As previously for the \( S_{ij} - S_i \) term, using the definition of \( S_{H_{ji}} \), we can write,

\[ S_{H_{ji}} - S_i = \sum_l \beta_{ji}^+ (S_{ji_l}^+ - S_i) \]  

(3.52)

where \( S_{ji_l}^+ \) is the value in the mesh element \( \Omega_{ji_l}^+ \), which belongs to \( w(j) \) by construction. Then, we need to assume that the following property holds,

**Hypothesis 3.4.1.** The elements \( \Omega_{ji_l}^+ \) chosen in order to compute the value \( S_{H_{ji}} \), which
belong to the \( w(j) \) neighborhood by construction, also belong to the \( w(i) \) neighborhood.

Now with this property, and introducing the notation,

\[
\mathcal{L}^+_{ji} = \{ \Omega^+_{ji} | l \in \mathbb{N} \}
\]

(3.53)

To denote the set of selected forward neighboring elements, we therefore get,

\[
(S_{Hji} - S_i) \frac{\psi_{ji}}{\eta_{ji}^+} = \sum_{k \in w(i)} \lambda_{ijk} (S_k - S_i)
\]

(3.54)

with \( \lambda_{ijk} = \frac{\psi_{ji}}{\eta_{ji}^+} \beta_{ji}^+ \) if \( \Omega_k \in \mathcal{L}^+_{ji} \), and \( \lambda_{ijk} = 0 \) if \( \Omega_k \notin \mathcal{L}^+_{ji} \). So, once again we do have the nonnegativity of the \( \lambda_{ijk} \) if the limiter is nonnegative. Besides, the sum reads in,

\[
\sum_{k \in w(i)} \lambda_{ijk} = \frac{\psi_{ji}}{\eta_{ji}^+}
\]

(3.55)

which will be uniformly bounded with an \textit{ad hoc} limiter. We finally get for the \( S_{ji} - S_i \) term,

\[
S_{ji} - S_i = (S_j - S_i) \left( 1 - \frac{\psi_{ji}}{\eta_{ji}^+} \right) + \sum_{k \in w(i)} \lambda_{ijk} (S_k - S_i)
\]

(3.56)

3.4.4 \textit{Second rewriting of the scheme}

Now, if we introduce in (3.40) the relations found for \( S_{ij} - S_i \) and \( S_{ji} - S_i \), then the scheme reads in,

\[
S_i^{n+1} = S_i^n + \sum_{j \in w(i)} \left( v_{ij}^- \left( 1 - \frac{\psi_{ji}}{\eta_{ji}^+} \right) (S_j - S_i) - v_{ij}^+ \sum_{k \in w(i)} \omega_{ijk} (S_i - S_k) \right)
\]

(3.57)

Afterwards, imposing \( v_{ij}^- = 0 \) if \( j \in w(i) \), \( j \notin v(i) \), allows to extend the sum on \( j \) over the set \( w(i) \) for the first term of the sum in relation (3.57). For the last two terms of the sum
on \( j \), we can permute the sums on \( j \) and \( k \). In the case of the second term, this means,

\[
\sum_{j \in v(i)} v^{-}_{ij} \sum_{k \in w(i)} \lambda_{ijk}(S_k - S_i) = \sum_{k \in w(i)} (S_k - S_i) \left( \sum_{j \in v(i)} \lambda_{ijk} v^{-}_{ij} \right)
\]

\[
= \sum_{j \in w(i)} (S_j - S_i) \left( \sum_{k \in v(i)} \lambda_{ikj} v^{-}_{ik} \right)
\]  \tag{3.58}

A similar result holds for the third term, so that the relation (3.57) becomes,

\[
S_{n+1}^i = S^n_i + \sum_{j \in w(i)} (S_j - S_i) \left( v^{-}_{ij} \left( 1 - \frac{\psi_{ji}}{\eta_{ji}} \right) + \sum_{k \in v(i)} (\omega_{ikj} v^+_i + \lambda_{ikj} v^-_{ik}) \right)
\]  \tag{3.59}

Therefore the scheme can finally be written under the following form,

\[
S_{n+1}^i = S^n_i + \sum_{j \in w(i)} c_{ij}(S_j - S_i)
\]  \tag{3.60}

where the coefficients \( c_{ij} \) read in,

\[
c_{ij} = v^{-}_{ij} \left( 1 - \frac{\psi_{ji}}{\eta_{ji}} \right) + \sum_{k \in v(i)} (\omega_{ikj} v^+_i + \lambda_{ikj} v^-_{ik})
\]  \tag{3.61}

### 3.4.5 Nonnegativity and boundedness of the coefficients

As mentioned in relation (3.39), the coefficients \( v^{-}_{ij} \) and \( v^+_i \) are nonnegative. Furthermore, if the limiter function is such that,

\[
\psi_{ij} \in [0, \eta^+_i] \quad j \in v(i)
\]  \tag{3.62}

then we get the nonnegativity of the coefficients \( c_{ij} \). Let us now write their sum,

\[
\sum_{j \in w(i)} c_{ij} = \sum_{j \in w(i)} v^{-}_{ij} \left( 1 - \frac{\psi_{ji}}{\eta_{ji}} \right) + \sum_{j \in w(i)} \sum_{k \in v(i)} (\omega_{ikj} v^+_i + \lambda_{ikj} v^-_{ik})
\]  \tag{3.63}
\[
\sum_{j \in \text{w}(i)} c_{ij} = \sum_{j \in \text{w}(i)} v_{ij}^- \left(1 - \frac{\psi_{ji}}{\eta_{ji}}\right) + \sum_{j \in \text{v}(i)} \left( v_{ij}^+ \left(\sum_{k \in \text{w}(i)} \omega_{ijk}\right) + v_{ij}^- \left(\sum_{k \in \text{w}(i)} \lambda_{ijk}\right)\right) \quad (3.64)
\]

Using relations (3.49) and (3.55), and because \(v_{ij}^- = 0\) if \(j \in \text{w}(i), j \notin \text{v}(i)\), we obtain,

\[
\sum_{j \in \text{w}(i)} c_{ij} = \sum_{j \in \text{v}(i)} v_{ij}^- \left(1 - \frac{\psi_{ji}}{\eta_{ji}}\right) + \sum_{j \in \text{v}(i)} \left( v_{ij}^+ \frac{\psi_{ij}}{\eta_{ij} r_{ij}} + v_{ij}^- \frac{\psi_{ji}}{\eta_{ji}}\right) \quad (3.65)
\]

And the sum finally reads in,

\[
\sum_{j \in \text{w}(i)} c_{ij} = \sum_{j \in \text{v}(i)} \left(v_{ij}^- + v_{ij}^+ \frac{\psi_{ij}}{\eta_{ij} r_{ij}}\right) \quad (3.66)
\]

Now we know that stability is conditioned by \(\sum c_{ij} \leq 1\), since the value \(S_{i+1}^n\) is thereby obtained as a convex combination between values within the \(\text{w}(i)\) neighborhood. This indeed complies with the DMP stated in (3.27) just by considering the \(w\)-like neighborhood as the set \(\mathcal{U}\) used in Definition 3.4.1. Introducing \(N_i = \text{card}(v(i))\), i.e. the number of edges of the element \(\Omega_i\), then from relation (3.66) we can derive two sufficient stability conditions,

\[
\text{if } v_{ij}^- \leq \frac{1}{2N_i}, \quad \text{and if } v_{ij}^+ \frac{\psi_{ij}}{\eta_{ij} r_{ij}} \leq \frac{1}{2N_i}, \quad \text{then } \sum_{j \in \text{v}(i)} c_{ij} \leq 1 \quad (3.67)
\]

Let us now introduce the parameters,

\[
N = \max_{\Omega_i} N_i, \quad h_0 = \min_{j \in \text{v}(i)} \frac{|\Omega_i|}{|E_{ij}|}, \quad M = \max_{t \in [0,T]} \left(\frac{\partial \psi_{ij}}{\partial S_1}(\tilde{S}_{ij}, S_i), -\frac{\partial \psi_{ij}}{\partial S_2}(S_{ij}, S_{ij}^*)\right) \quad (3.68)
\]

and let \(v_{\max}\) denote the maximum reachable CFL number, such that,

\[
v_{\max} = \Delta t M / h_0, \quad v_{ij}^- \leq v_{\max}, \quad v_{ij}^+ \leq v_{\max} \quad (3.69)
\]
Then the first condition in (3.67) is included in the uniform sufficient condition,

\[ \psi_{ij} \leq 2N_i^{+}v_{ij}^{+} \]  

which gives rise to a sufficient stability condition on the time step,

\[ \Delta t \leq \frac{h_0}{2MN} \]  

The second sufficient condition in (3.67) leads to a condition on the limiter,

\[ \psi_{ij} \leq \frac{\eta_{ij}^{-}r_{ij}}{2N_i^{+}v_{ij}^{+}} \]  

We can keep this condition as is, which will generate a CFL-dependent limiter. Or, using the fact that \(2N_i^{+}v_{ij}^{+} \leq 1\), we can derive another sufficient condition,

\[ \psi_{ij} \leq \eta_{ij}^{-}r_{ij} \]  

which will generate a more classical CFL-independent limiter.

3.4.6 Summary of the \(L^\infty\) stability proof

The finite-volume MUSCL scheme (3.29) based on the novel multislope reconstruction complies with the DMP stated in Definition 3.4.1 and therefore is \(L^\infty\)-stable, under the sufficient condition on the time step,

\[ \Delta t \leq \frac{h_0}{2MN} \]  

and under the CFL-dependent sufficient condition on the limiter function,

\[ 0 \leq \psi_{ij} \leq \min \left( \eta_{ij}^{+}, \frac{\eta_{ij}^{-}r_{ij}}{2N_i^{+}v_{ij}^{+}} \right) \]
in which is included a more classical CFL-independent sufficient condition on the limiter,

\[ 0 \leq \psi_{ij} \leq \min \left( \eta^+_{ij}, \eta^-_{ij} r_{ij} \right) \]  

(3.76)

Finally, the second-order consistency requires the following additional property of the limiter,

\[ \text{if } r_{ij} = 1 \text{ then } \psi_{ij} = 1 \]  

(3.77)

### 3.5 Flux limiter

In order for a high-resolution scheme to have monotonicity-preserving property, the limiter function should be designed to fulfil some boundedness criteria. For a uniform structured grid, Sweby’s TVD criterion can be adopted,

\[ 0 \leq \psi(r) \leq \min (2, 2r), \text{ } r \geq 0 \text{ and } \psi(r) = 0, \text{ } r < 0 \]  

(3.78)

The second condition is added as a safe treatment for extrema. The flux limiter schemes that lie in the Sweby’s diagram can be both second-order and TVD. Here we review several popular flux limiters in the CFD literature:

- **Minmod limiter:**

  \[ \psi(r) = \max [0, \min (r, 1)] \]  

(3.79)

- **Superbee limiter:**

  \[ \psi(r) = \max [0, \min (2r, 1), \min (r, 2)] \]  

(3.80)

- **Van Leer limiter:**

  \[ \psi(r) = \frac{r + |r|}{r + 1} \]  

(3.81)

- **Van Albada limiter:**

  \[ \psi(r) = \frac{r (r + 1)}{r^2 + 1} \]  

(3.82)
In general, the piecewise-linear flux-limiters (such as Minmod and Superbee) act simply as switches between different linear schemes and is highly flexible. However, the flux-limiters of this kind suffer from an adverse effect on nonlinear convergence behavior because of their discontinuous nature. Delis and Nikolos (2013) show that convergence problems are pronounced in the case of limiters that make use of nondifferentiable functions as the max and min ones. In contrast, the gradually-switching smooth limiters (such as Van Leer and Van Albada) exhibit better convergence behavior than the piecewise-linear flux-limiters at a price of accuracy. Zhang et al. (2015) developed a refined CFL-independent gradually-switching smooth flux-limiter (TCDF) for 1D uniform grid scenario through maximizing the region of a well-behaved linear scheme (third-order QUICK),

$$\psi(r) = \begin{cases} 
    r^3 - 2r^2 + 2r & \text{when } 0 \leq r < 0.5 \\
    0.75r + 0.25 & \text{when } 0.5 \leq r < 2 \\
    \frac{2r^2 - 2r - 9}{r^2 - r - 1} & \text{when } 2 \leq r
\end{cases}$$

(3.83)

Zhang et al. (2015) showed that TCDF has a better overall performance than the existing flux limiters in terms of accuracy and nonlinear convergence. The flux limiters presented above are plotted in Figure 3.6, where Sweby’s criterion is illustrated by the shaded region. The Minmod and Superbee limiters represent the lower and upper boundary of the second-order region, respectively.

We develop an adaptive flux limiter for the multislope MUSCL scheme to accommodate non-uniform and distorted unstructured grids. As shown in the previous section, the geometric ratio $\eta^-$ is fixed to the constant 2 in our scheme. This property leads to the following stability condition:

$$0 \leq \psi(r) \leq \min(\eta^+, 2r)$$

(3.84)

The developed limiter can smoothly switch between the QUICK scheme and the horizontal
boundary $\eta^+$. In this way the monotonicity property is strictly ensured without degradation of nonlinear convergence. For the other parts of the flux limiter, the TCDF scheme is employed, which results in a hybrid formula,

$$
\psi(r) = \begin{cases} 
    r^3 - 2r^2 + 2r & \text{when } 0 \leq r < 0.5 \\
    \frac{1}{\epsilon} \log \left( e^{\epsilon(0.75r+0.25)} + e^{\epsilon\eta^+} \right) & \text{when } 0.5 \leq r
\end{cases}
$$

(3.85)

where $\epsilon$ is a smoothing coefficient that depends on $\eta^+$,

$$
\epsilon = -15/\eta^+
$$

(3.86)

The adaptive limiter functions for $\eta^+ = 2$ and $\eta^+ = 1.5$ are plotted in Figure 3.7. It can be seen that a good compromise between maintaining accuracy and nonlinear convergence performance on non-uniform grids can be achieved with the newly developed limiter.

### 3.6 Lower-dimensional DFM discretization

The developed MFD-MUSCL framework is adapted to a lower-dimensional discrete
fracture-matrix model. The reservoir and fracture are modeled in two separate domains. Since fractures have an order of magnitude smaller length scale (fracture width) compared to reservoir, the boundary is represented as a lower dimensional surface (Ahmed et al. 2015). As mentioned in Matthai et al. (2010), although the lower-dimensional fracture representation allows the explicit scheme to significantly relax the CFL criterion, the ratio of cell length to velocity is still unfavorably small. Note that a small CFL in a fracture cell may cause the entire simulation to slow down. Therefore, the fully-implicit formulation adopted in this work is expected to efficiently circumvent the associated difficulty.

We apply the method called fracture cross flow equilibrium (FCFE) which is introduced by Hoteit and Firoozabadi (2008) to determine the boundary condition for fracture and matrix communication. Recent works of Zidane and Firoozabadi (2014), and Zidane and Firoozabadi (2016) present the implementations of the FCFE method on multicomponent and compositional flow problems. The pressure is assumed to be equal along the fracture width, and thus only the degree of freedom for fracture cell pressure is remained at the fracture-matrix interface. The schematic for FCFE concept is shown in Figure 3.8. As previously mentioned, in mimetic finite difference method the flux is written locally for all
faces within each gridcell. To assemble all the gridcells together, the continuity conditions for the flux and the pressure are imposed at each interface $E$ of two neighboring matrix gridcells $K$ and $K'$. We use $q_{K,E}^m$ for the mass flux of the matrix in the following discussions.

- If $E$ is neither a fracture nor a barrier, the continuity of flux and pressure is imposed.

\[
\begin{cases}
q_{K,E}^m + q_{K',E}^m = 0 \\
\pi_{K,E}^m = \pi_{K',E}^m
\end{cases}
\]  \hspace{1cm} (3.87)

- If $E$ is a fracture, the total flux across both sides of the matrix-fracture interface defines the transfer function $Q_E^f$ at $E$, which acts as a sink/source term. The continuity of the pressure across the fracture-matrix interface $E$ is imposed.

\[
\begin{cases}
q_{K,E}^m + q_{K',E}^m = Q_E^f \\
\pi_{K,E}^m = \pi_{K',E}^m = p_E^f
\end{cases}
\]  \hspace{1cm} (3.88)

- The flux and pressure at the domain boundaries are described by the Neumann or Dirichlet boundary conditions. If the interface $E$ is at the domain boundary then:

\[
\begin{cases}
q_{K,E}^m = q_E^N \\
\pi_{K,E}^m = \pi_E^D
\end{cases}
\]  \hspace{1cm} (3.89)
where \( \pi^D_E \) is a Dirichlet boundary condition, and \( q^N_E \) is a Neumann boundary condition. In this work, we assume an impermeable boundary and set \( q^m_{K,E} \) to be zero at the boundary.

For fracture intersection \( e \), we assume that the interface has a negligible volume, and thus no mass accumulation is considered. Similar continuity conditions as in Equation (3.87) is imposed at \( e \). The schematic for fracture intersection is shown in Figure 3.9.

\[
\begin{aligned}
\sum_{i=1}^{n_e} q^f_{K_i,e} &= 0 \\
\pi^f_{K_i,e} &= p^f_e 
\end{aligned}
\]  

(3.90)

where \( n_e \) is the number of fracture cells that connect to the intersection \( e \). \( p^f_e \) is the fracture intersection pressure.

For the high-resolution discretization of saturations in the DFM model, a simple treatment is employed. The saturation state at the matrix side is built in the same way as the scenario with no fracture. The state at the fracture side is just taken to be the fracture saturation, leading to a first-order approximation.

### 3.7 Results

Results will be presented for the immiscible two-phase flow with buoyancy forces.

#### 3.7.1 Validation

We validate the accuracy of the developed unstructured simulator against an in-
house black-oil simulator. The specification of the 2D synthetic model is shown in Table 5.1. The data of the base model is used for all the test cases, with modifications of some specific parameters. The correlations for rock and fluid compressibility, viscosity and density can be found in the user manual of the commercial simulator Eclipse. Quadratic relative-permeability functions are used: \( k_{rw} = S^2 \) and \( k_{ro} = (1 - S)^2 \). The associated PVT data of dead oil (PVDO) is shown in Table 4.2. The model has three fractures, as shown in Figure 3.10. An injector is placed at the bottom left corner and a producer at the top right. We compare the water saturation distributions at 400 days to examine the accuracy of the numerical model. The results for the Cartesian reference solution and unstructured high-order solution are plotted in Figure 3.11. The Cartesian model employs an explicit representation with logarithmic grid refinement for discrete fractures. The newly proposed multislope scheme with the adaptive flux limiter is used for the high-order solution. We also run the validation cases with the first-order scheme based on different resolutions of unstructured grid, as shown in Figure 3.12. The comparison results validate that the developed code are accurate. Although the difference in the overall solutions between the first-order and high-order schemes is negligible for this simulation scenario, improved resolutions in several detailed flow regions are still observed with the high-order scheme.

Figure 3.10: Fracture distribution
Table 3.1: Specification of the synthetic base model

<table>
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<th>Value</th>
<th>Unit</th>
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<tr>
<td>LX LY LZ</td>
<td>100 / 1 / 100</td>
<td>m</td>
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<td>psi</td>
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<td>Initial Porosity</td>
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<td>Water reference pressure</td>
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</tr>
<tr>
<td>Production BHP</td>
<td>1000</td>
<td>psi</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>400</td>
<td>day</td>
</tr>
</tbody>
</table>

Table 3.2: PVT data of dead oil (PVDO)

<table>
<thead>
<tr>
<th>Pressure</th>
<th>FVF</th>
<th>Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>1.012</td>
<td>1.16</td>
</tr>
<tr>
<td>1200</td>
<td>1.004</td>
<td>1.164</td>
</tr>
<tr>
<td>2000</td>
<td>0.996</td>
<td>1.167</td>
</tr>
<tr>
<td>2800</td>
<td>0.988</td>
<td>1.172</td>
</tr>
<tr>
<td>3600</td>
<td>0.9802</td>
<td>1.177</td>
</tr>
<tr>
<td>4400</td>
<td>0.9724</td>
<td>1.181</td>
</tr>
<tr>
<td>5200</td>
<td>0.9646</td>
<td>1.185</td>
</tr>
<tr>
<td>5600</td>
<td>0.9607</td>
<td>1.19</td>
</tr>
</tbody>
</table>

3.7.2 Numerical convergence

Grid convergence studies are performed for different numerical schemes. The base model is used but without fracture and gravity effect is neglected. Linear relative-permeability functions are employed. Water reference viscosity is changed to 1 cP. The total simulation time is 600 days with timestep size as 2 days. Because of the absence of an analytical solution for this case, coarse grid simulations are compared to a reference solution on a fine grid,
Figure 3.11: Water saturation distributions at 400 days for the Cartesian reference solution and unstructured high-order solution

(a) Cartesian  
(b) Unstructured High-order

Figure 3.12: Water saturation distributions at 400 days for unstructured first-order scheme based on different grid resolution assuming the fine-grid solution to be exact.

Simulations are performed on different levels of mesh refinement with the characteristic element size $h$ computed as $\sqrt{2V}$ for triangles, with $V$ the average element volume. To
obtain convergence rates, we compute the $L_2$ error over the entire domain as:

$$L_2 = \sqrt{\frac{1}{N} \sum_{j=1}^{N} (S_j^{\text{numerical}} - S_j^{\text{exact}})^2}$$ (3.91)

where $N$ is the number of uniformly generated sample points. For unstructured meshes, we need to interpolate the numerical solution between two different meshes to calculate the $L_2$ norm.

The $L_2$ errors of the different numerical schemes are plotted logarithmically versus the grid sizes $h$ in Figure 3.13, where the slopes provide the convergence rates. From the results we can see that the discretizations converge as the mesh is refined. The first-order solutions have considerably more numerical diffusion and less convergence rate than the higher-order solutions. As expected, the new multislope scheme with the adaptive limiter exhibits the highest accuracy. Note that the convergence rates of higher-order methods are quadratic on relatively fine grids, but the slopes decrease on the coarse grids.

Figure 3.14 shows the 1D results on a coarse grid for a vertical cross-section that runs diagonally from the injector at $(0,0)$ to the producer at $(100m, 100m)$. The higher-order schemes provide considerable improvement in the resolution of the saturation front compared with that of the first-order scheme.

Grid convergence is also examined with respect to time accuracy. The total simulation time is 400 days. The new multislope scheme with the adaptive limiter is used for obtaining high-order solutions. The reference solution is generated from the case on a fine grid and the timestep size $dt = 0.5$ day with CFL = 1 is used. Mesh refinements are studied for different timestep sizes and are plotted in Figure 3.15 (e.g. $dt = 2$” represents the solutions from the new multislope scheme with the adaptive limiter under CFL = 4 for the reference case). The first-order solutions are also provided with $dt = 0.5$ day. The results show the impacts of time accuracy on the solutions: the errors increase and convergence rates decrease with larger timestep sizes. For $dt = 10$ (CFL = 20 for the reference case), a low convergence rate is observed, indicating that the overall solution accuracy is dominated by the errors in the
time discretization (first-order backward Euler) under this simulation scenario. In practice, reasonable timestep sizes have to be chosen to ensure desirable solution accuracy. Note that the implicit discretization with large timestep sizes is more useful for the heterogeneous cases and discrete fractured reservoirs, where the CFL constraint of the entire domain is
determined by those few small elements (or low porosities). In such applications, we can safely increase the CFL number for the implicit scheme to orders of magnitude beyond the stability limit for the explicit scheme before the appearance of significant numerical diffusion (Lie et al. 2016).

![Grid convergence with respect to time accuracy](image)

**Figure 3.15:** Grid convergence with respect to time accuracy

### 3.7.3 Accuracy of high-resolution methods

We run numerical studies to examine the spatial accuracy of different high-resolution schemes. The base model with the distribution of discrete fractures shown in Figure 3.10 is used with the modifications of several properties and parameters: linear relative-permeability functions are employed; water reference viscosity is changed to 1 cP; the total simulation time is 600 days with timestep size as 2 days. Figure 3.16 shows the unstructured mesh. The water saturation contours obtained from the first-order scheme, the new multislope scheme with Van Albada and the adaptive limiter are shown in Figure 3.17. The first-order solution on a very fine grid is also presented. From the figures we can see that the first-order scheme suffers from excessive numerical diffusion, while the high-resolution schemes provide improved front resolution. The adaptive limiter provides slightly better solution than Van
Albada limiter. The result for Buffard and Clain’s multislope scheme is not presented here, because it is very similar with the results obtained from the new multislope scheme for this simulation scenario. However, Buffard and Clain’s method leads to much worse nonlinear convergence performance.

We run another case with different fracture configuration. The mesh and water saturation contours are shown in Figure 3.18. The higher-order method increases resolution significantly compared with the first-order method; the latter shows non-physical features in the numerical solution and leads to earlier water breakthrough in the producer.

3.7.4 Nonlinear convergence performance

We run the simulation case presented in the previous section to examine the nonlinear convergence of different numerical schemes. The unstructured mesh shown in Figure 3.16 is used. The total simulation time is 300 days and the other parameters are unchanged. We compare the new multislope scheme with different flux limiters to Buffard and Clain’s scheme. The nonlinear iteration performances and CPU time ratios are summarized in Table 3.3. The new multislope scheme is used as the high-order reconstruction for the numerical scheme only with limiter’s name (e.g. TCDF limiter). The results show that Buffard and Clain’s scheme leads to much more iterations, mainly due to the strict geometric constraints.
Figure 3.17: Water saturation contours for the first case

associated with the scheme. In comparison, the newly developed multislope scheme shows better convergence performance, especially for the adaptive flux limiter, which can strictly preserve the monotonicity property.

It can also be seen that the higher-order schemes are computationally more expensive than the first-order scheme. This is partly due to the increased nonlinearity of the discretised equations which require more iterations for convergence. Another reason is that the higher-order reconstruction procedure also exhibits stencil increases which result in ad-
Figure 3.18: Results for the second case

Additional fill-in and deterioration of matrix properties of the Jacobian. This degradation in computational performance can be alleviated by using an efficient iterative linear solver with proper preconditioning. The investigation on the linear solution techniques is beyond the scope of this paper and is subject to a future work. It should be noted that although the higher-order schemes require more CPU time than the first-order scheme for a given mesh, the higher-order schemes can still be orders of magnitude more efficient than the first-order scheme from the aspect of grid convergence rate.

We run another case with quadratic relative permeability and initial water saturation
Table 3.3: Nonlinear iteration performance and CPU time ratio

<table>
<thead>
<tr>
<th>Numerical scheme</th>
<th>Timestep size (day)</th>
<th>CPU time ratio with 10 days timestep size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Buffard and Clain’s method with Van Albada limiter</td>
<td>730 863 440</td>
<td>2.83</td>
</tr>
<tr>
<td>TCDF limiter</td>
<td>694 338 201</td>
<td>1.48</td>
</tr>
<tr>
<td>Van Albada limiter</td>
<td>672 315 178</td>
<td>1.31</td>
</tr>
<tr>
<td>Adaptive limiter</td>
<td>689 336 200</td>
<td>1.46</td>
</tr>
<tr>
<td>First-order</td>
<td>667 287 167</td>
<td>1.0</td>
</tr>
</tbody>
</table>

changed to 0.1. Water reference viscosity becomes 0.2 cP. Injection rate is 100 m³/D, and total simulation time is 300 days. The nonlinear iteration performances of the newly developed multislope scheme with different flux limiters are summarized in Table 3.4. In this case, the impact of the monotonicity preserving property on nonlinear convergence is clearly observed. Violation of the stability condition may cause oscillations in the solutions as well as in the iterative behavior. Compared with the conservative Van Albada limiter, the adaptive limiter can achieve a balance between accuracy and convergence performance. In the third case, production BHP is changed to 2000 psi, and the results are summarized in Table 3.5.

Table 3.4: Iteration performance of the second case

<table>
<thead>
<tr>
<th>Timestep size (day)</th>
<th>2</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDF</td>
<td>956</td>
<td>789</td>
<td>665</td>
</tr>
<tr>
<td>VanLeer</td>
<td>832</td>
<td>419</td>
<td>450</td>
</tr>
<tr>
<td>VanAlbada</td>
<td>812</td>
<td>384</td>
<td>384</td>
</tr>
<tr>
<td>Adaptive</td>
<td>853</td>
<td>424</td>
<td>460</td>
</tr>
</tbody>
</table>

Table 3.5: Iteration performance of the third case

<table>
<thead>
<tr>
<th>Timestep size (day)</th>
<th>2</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDF</td>
<td>851</td>
<td>625</td>
<td>405</td>
</tr>
<tr>
<td>VanLeer</td>
<td>836</td>
<td>418</td>
<td>263</td>
</tr>
<tr>
<td>VanAlbada</td>
<td>820</td>
<td>387</td>
<td>258</td>
</tr>
<tr>
<td>Adaptive</td>
<td>850</td>
<td>421</td>
<td>308</td>
</tr>
</tbody>
</table>
3.7.5 Further simulation runs

We perform a further simulation test using the base model with a complex fracture network and linear relative-permeability functions. The timestep size is set to 1 day, and the injection rate is 400 m$^3$/D. The unstructured mesh for the fracture network and water saturation profiles at 400 days are shown in Figure 3.19. The newly proposed multislope scheme with the adaptive flux limiter provides a better overall resolution of the saturation fronts compared to the first-order scheme.

Figure 3.19: Results for the case with complex fracture network
CHAPTER 4
IMPROVED PROJECTION-BASED EMBEDDED
DISCRETE FRACTURE MODEL (PEDFM)

4.1 EDFM: review and analysis

4.1.1 Multiphase flow

The mass-conservation equations for the phases are:

$$\frac{\partial}{\partial t} (\phi \rho \alpha S \alpha) + \nabla \cdot (\rho \alpha u \alpha) = q_{f \alpha}^m + q_{W \alpha}^W$$  (4.1)

where $\phi$ is porosity. $S \alpha$, $\rho \alpha$, and $u \alpha$ are saturation, density and velocity of each phase. $q_{f \alpha}^m$ denotes the mass communication between the fracture and matrix domains, and it has the similar expression as flux term. $q_{W \alpha}^W$ is well flow rates (source and sink terms). Here we focus on the model of immiscible two-phase flow with the oil (nonwetting) and the water (wetting) phases ($\alpha = o, w$). Note that although all the presented examples are based on this simplified model, the new method developed can be readily applied to more complex systems with multiphase multicomponent (compositional) fluids.

4.1.2 EDFM

For a DFM method, removing the constraint of mesh conformity can be convenient in realistic cases with numerous and complex fractures. The concept of EDFM is to split a fractured medium into a separate matrix and fracture mesh (see Figure 4.1) and to couple them through a transfer function. The embedded fractures are discretized vertically and horizontally by the cell boundaries. This ensures that each matrix gridblock cut by fractures

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contains exactly one fracture cell per fracture. In this chapter, all the model implementations are 2D. It is assumed that reservoir formation is fully penetrated by vertical fractures.

Figure 4.1: Schematic of matrix and fracture meshes in EDFM. The matrix is considered as a background mesh. Each fracture cell is represented by two blue dots and the green dots indicate fracture intersections which are not geometric constraints.

A standard finite-volume scheme is employed to discretize the fluid flow problem. A two-point flux approximation (TFPA) is used to approximate the flux at a cell interface. The degrees of freedom for a pressure and a saturation variable are assigned to each matrix cell and each fracture cell. The three kinds of connection provided by EDFM for the flux terms are as follows: 1) between a fracture segment and the matrix block it penetrates. 2) between fracture segments of an individual fracture. 3) between intersecting fracture segments.

EDFM applies the concept of wellbore index (WI) to derive a transport index for the fracture-matrix ($f - m$) connection. The transmissibility is given by:

$$T_{fm} = \frac{kA}{\langle d \rangle}$$  \hspace{1cm} (4.2)

where $A$ is the fracture surface area contacted with the matrix the gridblock. $k$ is the harmonic average for the permeability of fracture and matrix and is close to the matrix permeability in most cases. Li and Lee (2008) assume that the pressure around fracture is linearly distributed, and with this approximation the average normal distance $\langle d \rangle$ from the
fracture in the gridblock can be computed as:

$$\langle d \rangle = \frac{\int \mathbf{n} \cdot x \, dV}{V} \quad (4.3)$$

where \( \mathbf{n} \) is the unit normal vector pointing to the fracture face. \( x \) is the distance from the fracture; \( dV \) and \( V \) are the volume element and volume of the gridblock, respectively. The integral can be calculated numerically in a preprocessing code. Now the mass transfer of phase \( \alpha \) between fracture and matrix is:

$$\Psi_{f\alpha} = T_{f\alpha} \frac{k_{f\alpha}}{\rho_{\alpha}} (p_f - p_m) \quad (4.4)$$

The mass transfer terms of the other two connections can be calculated in a similar way as Equation (4.4). For a connection between two cells of an individual fracture, \( k \) is fracture permeability in the transmissibility; \( d \) is the distance between the centers of two fracture segments, and \( A \) is the fracture aperture times the length of the intersection line.

The transmissibility for a connection between two intersecting fracture cells is derived based on the star-delta transformation presented by Karimi-Fard et al. (2004):

$$T_{ff} = \frac{T_{f1} T_{f2}}{T_{f1} + T_{f2}} \quad (4.5)$$

$$T_{f1} = \frac{k_{f1} w_{f1} L_{int}}{d_{f1}}, \quad T_{f2} = \frac{k_{f2} w_{f2} L_{int}}{d_{f2}} \quad (4.6)$$

where \( L_{int} \) is the length of the intersection line bounded in the matrix gridblock. \( w_f \) is fracture aperture. \( d_f \) is the weighted average of normal distances from the center of the fracture subsegments (on each side of the intersection line) to the intersection line. Readers could refer to Moinfar et al. (2013) for more details regarding the computations of the connection transmissibilities.
4.1.3 Analysis

Here we present a detailed analysis of the flow process for the water displacement across a single fracture to illustrate the limitation of the EDFM method. Figure 4.2 shows a comparison between EDFM and the realistic (physical) flow scenario. Consider a water front moving from the right to the left. During the realistic flow process, water will first flow inside the matrix cell $m_2$ and enter the fracture; then the flux is split into two parts: along (cyan arrows) and across (green arrows) the fracture. In contrast, for EDFM the fracture acts as a sink term in $m_2$ and a large fraction of the injected fluid could be sucked into the fracture, resulting in an unphysical flux split and thus a lower saturation value of $m_2$. The flux across the surface between $m_1$ and $m_2$ becomes less because the phase mobility is evaluated at the upstream cell $m_2$. In other words, the realistic process should always exhibit the flow across the fracture from one side to the other. EDFM has the limitation that the fluxes on the two sides cannot be calculated separately, and thus the fluid tends to focus along the fracture as a preferential path.

![Figure 4.2: Comparison of the flow process between EDFM and the realistic scenario](image)

We consider a simple example to illustrate how much error the EDFM method can cause in the scenario of multiphase flow. The specification of the 2D synthetic model is shown in Table 5.1. The data of the base model will also be used for all the rest of test cases, with
modifications of some specific parameters. The correlations for rock and fluid compressibility, viscosity and density can be found in the user manual of the commercial simulator Eclipse. Quadratic relative-permeability functions are used: $k_{rw} = S^2$ and $k_{ro} = (1 - S)^2$. The associated PVT data of dead oil (PVDO) is shown in Table 4.2.

Time discretization is carried out using a backward, first-order Euler scheme. The fully-implicit discretization of a cell in the matrix domain can be written as,

$$\frac{\mid \Omega \mid}{\Delta t} \left[ (\phi \rho_s S_s)^{n+1} - (\phi \rho_s S_s)^n \right] + \sum_{E} F_{\alpha,E} = \Psi_{\alpha}^{m} + Q_{\alpha}^{W} \quad (4.7)$$

where we drop the superscript $(n+1)$ in the flux and well terms. $E$ denotes the interface between two neighboring gridcells $i$ and $j$.

Table 4.1: Specification of the synthetic base model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NX NY</td>
<td>50 / 50</td>
<td></td>
</tr>
<tr>
<td>LX LY</td>
<td>100 / 100</td>
<td>m</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>1</td>
<td>m</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2500 psi</td>
<td></td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>Initial Porosity</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>Rock compressibility</td>
<td>0.00034</td>
<td>1/psi</td>
</tr>
<tr>
<td>Rock reference pressure</td>
<td>2500 psi</td>
<td></td>
</tr>
<tr>
<td>Water reference pressure</td>
<td>3600 psi</td>
<td></td>
</tr>
<tr>
<td>Water reference viscosity</td>
<td>0.52341</td>
<td>cP</td>
</tr>
<tr>
<td>Water compressibility</td>
<td>4E-06</td>
<td>1/psi</td>
</tr>
<tr>
<td>Water viscosibility Cvw</td>
<td>1.2E-6</td>
<td>1/psi</td>
</tr>
<tr>
<td>Water reference density</td>
<td>63.02 lb/ft3</td>
<td></td>
</tr>
<tr>
<td>Oil reference density</td>
<td>30</td>
<td>lb/ft3</td>
</tr>
<tr>
<td>Fracture aperture</td>
<td>1E-03</td>
<td>m</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>1E-15 m2</td>
<td></td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>1E-10 m2</td>
<td></td>
</tr>
<tr>
<td>Injection rate</td>
<td>50</td>
<td>m3/D</td>
</tr>
<tr>
<td>Production BHP</td>
<td>1000</td>
<td>psi</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>400 day</td>
<td></td>
</tr>
</tbody>
</table>

The base model contains one vertical fracture, as shown in Figure 4.3(a). An injector is placed at the bottom right corner and a producer at the top left. We compare the water
Table 4.2: PVT data of dead oil (PVDO)

<table>
<thead>
<tr>
<th>Pressure</th>
<th>FVF</th>
<th>Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>1.012</td>
<td>1.16</td>
</tr>
<tr>
<td>1200</td>
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<tr>
<td>2800</td>
<td>0.988</td>
<td>1.172</td>
</tr>
<tr>
<td>3600</td>
<td>0.9802</td>
<td>1.177</td>
</tr>
<tr>
<td>4400</td>
<td>0.9724</td>
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<td>1.185</td>
</tr>
<tr>
<td>5600</td>
<td>0.9607</td>
<td>1.19</td>
</tr>
</tbody>
</table>

saturation profiles at 400 days obtained from EDFM against the model based on a logarithmic grid refinement (LGR) around the discrete fracture to examine the accuracy of the EDFM method. The LGR model employs an explicit representation for fractures and thus can be viewed as the reference. The water saturation profiles are plotted in Figure 4.3. From the results we can see that the existence of fracture results in strong heterogeneity and anisotropy, which have a great influence on the fluid flow. Large differences in the displacement profile between the two methods are observed. Specifically, for EDFM the water saturation values at the left side of the fracture are lower and more injected water flows out from the fracture top. This indicates that with EDFM the fluid moves more rapidly along the fracture than across it when the fluid front encounters the fracture conduit. The phenomena can be explained through the schematic for the flow process of EDFM shown in Figure 4.2.

Note that the above-mentioned limitation of EDFM will have a significant impact on saturation profile only for the scenario of the multiphase displacement across fractures. This argument can be supported by the simulation case with a diagonal fracture. The EDFM solutions are compared with the solutions obtained from a high-resolution cell-centered finite-volume (CCFV) framework that is recently developed by our research group (Jiang and Younis 2017). The framework employs a lower-dimensional DFM model that is based on an unstructured conforming grid. A consistent discretization scheme called mimetic finite difference (MFD) is used to approximate the phase velocities. The details of the numerical framework are summarized in the Appendix. Here the unstructured DFM solution is
Figure 4.3: Mesh and water saturation profiles of the base case generated using a first-order method (single-point upstream weighting) for approximating the phase mobilities. The results for the 2nd case are shown in Figure 4.7. A satisfactory match of the saturation profile between the two models can be observed. Clearly, EDFM is ideally designed for the single-well depletion and injection processes where fluids flow simultaneously out of (or into) fractures. The fracture-matrix transfer functions in EDFM can accurately capture the net fluxes through a fracture when the fracture acts as a single source (or sink) term.

Moreover, we observe that large inaccuracies from EDFM will only occur when there are asymmetries or anisotropies in the flow field around fractures. Figure 4.7 shows the
water saturation profiles of the base case with different well locations. In order to obtain a symmetric water displacement profile, the well positions are changed to the center of the left and right reservoir boundaries. We can see that EDFM produces the solution with a reasonable accuracy compared with LGR. For this particular case, most of the injected fluid flows across the fracture instead of along the fracture conduit.

### 4.2 The improved pEDFM method

From the analyses conducted in the last section we expect that a method which can separately calculate the fluxes across the two sides of a fracture is highly desirable.
Also the method should properly determine the flux split to obtain an accurate multiphase displacement profile. One possible direction to proceed is adding more $f - m$ connections to handle the flux jump at the two sides of a fracture. However, the extended flux needs to be carefully designed. We first present a case to illustrate that unphysical flux connections may cause detrimental effects on solution accuracies. The base model shown in Figure 4.3 (a) is still used, but the fracture position is shifted to be aligned with a gridline so that the fracture is connected with the two neighboring matrix cells. Furthermore, the connection between the two matrix cells is allowed. The water saturation profile is plotted in Figure 4.6. It can be observed that the influences of the fracture are largely reduced due to the unphysical matrix-matrix ($m - m$) connections across the fracture.

Here we focus on the recently proposed pEDFM method (Tene et al. 2016) which is based on the introduction of additional $f - m$ flux connections. The previous analyses motivate us to exploit pEDFM as a promising method to resolve the limitations associated with EDFM. Again we examine the flow process for the water displacement across a single fracture. Figure 4.7 shows a comparison between pEDFM and the realistic (physical) flow scenario. From Figure 4.7 (a) we can see that the original matrix-matrix $m_2 - m_3$ connection in EDFM is replaced with a $f - m$ connection between the fracture and $m_3$. The flow sequence across the fracture is forced to be first into the fracture and from the fracture.

Figure 4.6: Water saturation profiles of the base case with different well locations
to \( m_2 \), then from \( m_2 \) to \( m_1 \). In this way, the limitation of EDFM that the fluxes on the two sides cannot be calculated separately is overcome. Under the extended formulation, more fluid will enter \( m_2 \), leading to higher flux rate across the \( m_1 - m_2 \) interface. We expect that a more physical split of fluxes can be achieved through pEDFM and the artificial flow sequence can be a good approximation for the realistic flow scenario.

Figure 4.7: Comparison of the flow process between pEDFM and the realistic scenario

Now we review the formulae of connection transmissibility for pEDFM by considering a more general case, shown in Figure 4.8. The 2D case contains a fracture \( f \) that is partially
interacted with the matrix cell \( m_i \). \( m_i \) has two neighboring matrix cells \( m_j \) and \( m_k \). Let \( A_{f m_i} \) be the area of the fracture segment in the matrix cell. The areas of the fracture projections in the X and Y directions are \( A_{f m_i}^{pX} \) and \( A_{f m_i}^{pY} \), respectively. The projected fracture segments can serve as the measure to determine the extended \( f - m \) connections. Only the matrix cells that are nearer to the fracture segment along each direction will be selected. The transmissibilities for the \( f - m \) connections are given as:

\[
T_{f m_i} = \frac{k_{f m_i} A_{f m_i}}{\langle d \rangle_{f m_i}} \tag{4.8}
\]

\[
T_{f m_j} = \frac{k_{f m_j} A_{f m_i}^{pX}}{d_{f m_j}}, \quad T_{f m_k} = \frac{k_{f m_k} A_{f m_i}^{pY}}{d_{f m_k}} \tag{4.9}
\]

where \( \langle d \rangle_{f m_i} \) is the average normal distance. \( d_{f m_j} \) and \( d_{f m_k} \) are the distances from the centers of \( m_j \) and \( m_k \) to the center of the fracture segment. While adding the extra \( f - m \) connections, the \( m - m \) connections need to be modified correspondingly because parts of matrix flow area are blocked by the fracture. The transmissibility for the connection between \( m_i \) and \( m_j \), for example, is calculated as:

\[
T_{ij} = \frac{k_{ij} \left( A_{ij} - A_{f m_i}^{pX} \right)}{d_{ij}} \tag{4.10}
\]

where \( A_{ij} \) is the area of the interface shared by \( m_i \) and \( m_j \). \( d_{ij} \) is the distance between the centers of the two cells. The effective flow area of \( m - m \) is the original interface area minus the projected area of the fracture segment, and will become zero if the fracture fully cuts through the matrix cell. It can be seen that two extra \( f - m \) connections per fracture cell will be created for a 2D Cartesian grid. The above \( T \) formulae are provided in the pEDFM approach proposed by Tene et al. (2016). We note here that pEDFM is originally designed for accurately modeling the effect of the lower-dimensional features with a wide range of permeabilities (e.g. flow barriers).

In the following contents we will present one extension and two improvements for the
pEDFM approach. First a generalized formula for the effective flow area of $m - m$ connection under the scenario with multiple fracture segments in a matrix cell is given. The illustration case is shown in Figure 4.9. $A^p_{ij}$ and $A^p_{ik}$ are the total areas of the projected areas from the fracture segments onto the matrix-matrix interfaces. Consider the interface between $m_i$ and $m_j$, $A^p_{ij}$ is the union of the sets for the projected areas from the fracture segments that belong to $m_i$ and $m_j$:

$$A^p_{ij} = \overline{A_i} \cup \overline{A_j}$$  \hspace{1cm} (4.11)

where,

$$\overline{A_i} = \bigcup_{l=1}^{n_i} A^{X_{bm_i}}_{f_{lm_i}} , \hspace{1cm} \overline{A_j} = \bigcup_{l=1}^{n_j} A^{X_{lm_j}}_{f_{lm_j}}$$  \hspace{1cm} (4.12)

where $n_i$ and $n_j$ are the numbers of the fracture segments in $m_i$ and $m_j$, respectively.

We make an improvement upon pEDFM to accomodate the heterogeneity in matrix permeability. An illustration case is plotted in Figure 4.10. Matrix cell $m_i$ has ultra-low permeability so that a large permeability contrast is created between $m_i$ and $m_j$. In this case, the transmissibility for the extended $f - m$ connection needs to be specially calculated. For instance, consider fluid flowing from the left to the right. In reality, little fluid will enter the fracture conduits, due to the ultra-low permeability of $m_i$. However, artificial flow connections will be established and fluid will unphysically flow from $m_j$ into the fractures,
if face permeability $k_{fm_j}$ in Equation (4.9) is simply evaluated using the harmonic average between $m_j$ and the fractures. A proper way for calculating $T_{fm_j}$ is to first get the harmonic average $T_{m_im_j}$ between $m_i$ and $m_j$, and then perform harmonic averaging again for $T_{m_im_j}$ with $T_f$:

$$T_{fm_j} = \frac{T_{m_im_j}T_f}{T_{m_im_j} + T_f} \quad (4.13)$$

Using this formula $T_{fm_j}$ will become zero if the permeability of $m_i$ is zero.

Now we run some simulation cases to test the performances of pEDFM. Again the base case is considered and the results are plotted in Figure 4.11. A perfect match between the solutions obtained from pEDFM and the reference models is observed, indicating that
the method is accurate for this fracture configuration. However, in the next example we will illustrate that with a naive implementation of pEDFM, some undesirable degradations in numerical solutions may occur. The 2nd case shown in Figure 4.7 is employed and the water saturation profiles are compared in Figure 4.12. We can clearly see the incorrect values appeared around the fracture.

![Figure 4.11: Water saturation profiles of the base case](image)

We will present a simple but effective improvement upon the implementation of pEDFM. The limitation associated with the naive implementation is first analysed through examining the extended $f-m$ connections provided in the preprocessing part. The schematic of the extended $f-m$ connections created for the fracture configuration in the 2nd case is plotted in Figure 4.13(a). Here the fracture projections (green lines) are introduced as
an indicator for identifying which matrix cells are connected to the fracture in an extended $f - m$. It can be clearly seen that an abnormal configuration of the extended connections is created in the naive implementation. Such an unphysical configuration can result in a certain type of artificial flow barriers that affects the fluid flow in matrix. This explains why the incorrect saturation values are generated around the fracture in the 2nd case.

We notice that an unphysical configuration will only arise in the case where the distances between a fracture segment and the two neighboring matrix cells along one direction are the same. An arbitrary selection of the connected matrix cell will lead to unexpected errors in numerical solutions. The way to resolve this implementation issue is to impose some
constraints on the preprocessing stage for creating the extended connections. For example, the projection plotted in Figure 4.13(b) could be a proper choice. Some other examples are shown in Figure 4.14. An effective criterion to avoid unphysical connections is that the two projected lines of a fracture segment are not allowed to intersect with the fracture line on the same side. Figure 4.15 shows the connection list dependency of improved pEDFM in the computational domain for an example with two intersecting fractures.

In practice, the improved pEDFM method can be quite simple to implement. Basically, the original numerical code for EDFM does not need to be altered; only the preprocessing part for preparing connection lists is required to accommodate the new method. The program can first loop through all the fracture segment cells, to generate the extended $f - m$
connections for each fracture cell, one along each grid dimension. Simultaneously, the associated transmissibilities are calculated, and the extended connection information is added to the original \( f - m \) connection list. All the phase dependent properties (e.g. upstream weighting) will be handled in the same way by the simulator. For the \( m - m \) connections, a face-by-face calculation process can be employed. The ratio for the effective flow area of an interface shared by \( m_i \) and \( m_j \) is defined as:

\[
\beta_{ij}^A = \frac{A_{ij} - A_{ij}^p}{A_{ij}} \tag{4.14}
\]

where \( A_{ij}^p \) is the union of the projected areas from the neighboring fracture segments onto the interface. Then the transmissibilities in the \( m - m \) connection list will be multiplied by the corresponding area ratios. The 2nd test case is simulated one more time to compare the different methods and the results are plotted in Figure 4.16. We can see that the improved pEDFM method can replicate the solutions obtained from the reference models with acceptable accuracy.

### 4.3 Model verifications

We present several test cases with different fracture distributions to benchmark the performances of the new EDFM method for multiphase flow. Grid convergence studies are also performed for different numerical schemes. Coarse grid simulations are compared to a reference solution on a fine grid, assuming the fine-grid solution to be exact. Simulations are performed on different levels of mesh refinement with the characteristic element size \( h \) computed as \( \sqrt{V} \), with \( V \) the average element volume. To obtain convergence rate, we compute the \( L_2 \) error over the entire domain as:

\[
L_2 = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left( S_j - S_{j}^{ref} \right)^2} \tag{4.15}
\]

where \( S_j \) are the saturation values from the coarse simulations. \( N \) is the number of uniformly
Figure 4.16: Water saturation profiles of the 2nd case

generated sample points. For unstructured meshes, we need to interpolate the numerical solutions between two different meshes to calculate the $L_2$ norm. The $L_2$ errors of the different numerical schemes are plotted logarithmically versus the grid sizes $h$, where the slopes provide the convergence rates. The results based on the high-resolution CCFV framework (Jiang and Younis 2017) are also presented as reference solutions. The newly proposed multislope scheme with the adaptive flux limiter is used for the second-order solutions. The details are summarized in the Appendix. In the following result sections, ”pEDFM with unphysical connections” indicates the method with the naive implementation, and ”Improved pEDFM” indicates the method with the physical constraint on the preprocessing for creating the extended connections. In summary, the comparison results of all the cases demonstrate that
the developed pEDFM method significantly outperforms the original EDFM method.

4.3.1 The base case

The convergence rates are plotted in Figure 4.17. From the results we can see that improved pEDFM has higher accuracy and convergence rate than EDFM. Compared to the first-order convergence rate of the improved pEDFM and unstructured DFM methods, EDFM shows an almost zeroth-order convergence. In addition, improved pEDFM has a similar performance with the unstructured DFM method, which is very desirable for an embedded type of method. Figure 4.18 shows the water saturation profiles of two different levels of grid resolution. The limitation of EDFM that cannot compute separately the exchange fluxes on the two sides of fracture is clearly observed. The region in the EDFM solutions that exhibits incorrect saturation values does not go away as the grid is refined, indicating that EDFM essentially is an unphysical numerical method.

![Figure 4.17: L_2 error norm versus grid size h of the base case](image)

Figure 4.17: L_2 error norm versus grid size h of the base case
4.3.2 Case 3

Figure 4.18 shows the water saturation profiles of two different levels of grid res-
olution. The comparisons among the different methods are shown in Figure 4.19. While EDFM generates the solution profile with large discrepancies, a good agreement is observed between improved pEDFM and the reference solution (Unstructured DFM). The unphysical fluxes in EDFM can lead to the more dominating effects of fractures: most of the fluid tends to flow along the fracture conduits. Incorrect solutions (e.g. asymmetric profile) can also be produced from pEDFM with unphysical connections. The convergence rates plotted in Figure 4.20 further confirm the accuracy of improved pEDFM. In this case, EDFM gives a worse convergence performance (zeroth-order). Figure 4.21 shows the water saturation profiles of two different levels of grid resolution.

4.3.3 Case 4

The water saturation profiles of the 4th case are shown in Figure 4.22.

4.3.4 Case 5

The water saturation profiles of the 5th case are shown in Figure 4.23.

4.3.5 Case 6

The water saturation profiles of the 6th case at 200 days are shown in Figure 4.24. In Figure 4.25 we also present the results of the case with linear relative permeability functions for matrix and fracture.

4.3.6 Case 7

The water saturation profiles of the 7th case are shown in Figure 4.26.

4.3.7 Case 8

The water saturation profiles of the 8th case are shown in Figure 4.27. The results of the case with linear relative permeability functions for matrix and fracture are also presented in Figure 4.28.
Figure 4.19: Mesh and water saturation profiles of the 3rd case
Figure 4.20: $L_2$ error norm versus grid size $h$ of the 3rd case
Figure 4.21: Water saturation profiles of the 3rd case
Figure 4.22: Mesh and water saturation profiles of the 4th case
Figure 4.23: Mesh and water saturation profiles of the 5th case
Figure 4.24: Mesh and water saturation profiles of the 6th case at 200 days
Figure 4.25: Water saturation profiles of the 6th case with linear relative permeabilities
Figure 4.26: Mesh and water saturation profiles of the 7th case
Figure 4.27: Mesh and water saturation profiles of the 8th case
Figure 4.28: Water saturation profiles of the 8th case with linear relative permeabilities
CHAPTER 5

COUPLED FLOW AND GEOMECHANICS MODELING

5.1 Gas flow and storage in deforming fractured shale

Shale gas sediments contain high concentration of organic material that are characterized by pores having sizes in the range from 1 to 100 nm. Because of the tiny pore space (nanometer scale), the internal surface area associated with the organic nanopores is very large. The organic material also exhibits greater adsorption potential for the hydrocarbon fluids compared to the conventional reservoirs. Therefore the organic pores are the ideal places for massively trapping gas in the adsorbed and dissolved states. Release of adsorbed gas has to be incorporated into a numerical model for accurately predicting reservoir performance (Wang and Marongiu-Porcu 2015).

As the geometric-length scale of the shale pores is comparable to the mean free path of the gas molecules, gas rarefaction effects including velocity slippage and Knudsen diffusion become significant, due to the strong rock-fluid interactions. This leads to deviation from continuum flow, and classical Darcy’s equation could not adequately describe the relevant non-viscous gas flow regimes (Javadpour et al. 2007). To quantify this type of non-Darcy mechanisms, the apparent permeability corrections are usually integrated into the standard Darcy’s equation. The apparent gas permeability is a function of Knudsen number, which is the ratio of the molecular mean free path to the hydraulic radius of the pores, and can be applied to characterize the various flow regimes. In addition, gas flow is affected by the adsorbed layer within the flow channels. The adsorbed molecules can potentially occupy much of the area available to flow. The reduction of the effective hydraulic radius will impact the non-Darcy gas flow, and thus should be considered in calculating the apparent permeability of the organic pores (Wei et al. 2016).
In conventional reservoirs, the stress-sensitivity of rock porosity and permeability generally has insignificant effects and is neglected in numerical simulation most of the time. However, for shale reservoirs, the ultra-low permeability of rock and abnormally high pore pressure can result in a remarkable impact of rock deformation, which needs to be properly taken into account (Huang and Ghassemi 2015). During gas depletion, the reduction of pore pressure causes a rise in the effective stress which, in turn compacts the reservoir and reduces its porosity and intrinsic permeability (Wang 2016). Meanwhile, gas desorption induces matrix shrinkage and retards the influences of the effective stress increase on pore properties (Cao et al. 2016). The net change in gas permeability is thus controlled by the competitive effects of declining pore pressure and sorption-induced matrix deformation. For dual-porosity systems, the pressure decline will cause fracture closure and the corresponding reduction in fracture conductivity (Liu et al. 2011). The matrix shrinkage may widen fracture aperture, leading to conductivity enhancement.

A unified apparent-permeability model is implemented to accurately capture the combined impacts of the non-Darcy flow, variations of the adsorbed layer and pore-structure alterations on matrix permeability.

5.1.1 Desorption

It has been shown that shale formation contains the organic-inorganic configuration: tiny organic kerogen is scattered through predominantly inorganic matters (Ambrose et al. 2011). Here the mass transfers from the adsorbed and free phase in organic nanopores are treated as a single source term which feeds the inorganic pore system. The source feeding behavior is approximated by the Langmuir isotherm model. The molar quantity of gas molecules adsorbed on the pore wall of organic material in shale is:

\[ m_g = \rho_R \rho_{gs} V_E \] (5.1)
The standard volume of gas adsorbed per unit rock mass can be expressed as:

$$V_E = \frac{pV_L}{p + P_L}$$  \hspace{1cm} (5.2)

where \(p\) is gas pressure; \(V_L\) is the Langmuir volume (the maximum adsorption capacity at a given temperature); \(P_L\) is the Langmuir pressure (the pressure at which the adsorbed gas content is equal to \(V_L/2\)); \(\rho_R\) is the rock bulk density; \(\rho_g\) is the gas molar density at standard condition, kmol/m\(^3\); \(V_E\) is the adsorption isotherm function.

### 5.1.2 Porosity and intrinsic permeability of matrix

The mechanical response of poroelastic medium is described by the Biot theory. Assuming small deformation and linear elasticity, the constitutive relationship for rock deformation and sorption is obtained by making an analogy between poroelastic dilation and thermal contraction (Huang and Ghassemi 2015). The effective stress law is:

$$\sigma_{ij} = \sigma'_{ij} - \alpha p \delta_{ij}$$  \hspace{1cm} (5.3)

where \(\sigma'_{ij}\) is effective stress:

$$\sigma'_{ij} = \left( K - \frac{2G}{3} \right) \varepsilon_{kk} \delta_{ij} + 2G \varepsilon_{ij} - K \varepsilon_s \delta_{ij}$$  \hspace{1cm} (5.4)

where \(\alpha = 1 - K/K_s\) is the Biot coefficient; \(G\) represents the shear modulus of shale; \(K_s\) is the bulk modulus of solid constituent; \(K = E/3 (1 - 2\nu)\) is the bulk modulus of solid skeleton; \(E\) denotes the Young’s modulus and \(\nu\) the Possion’s ratio. The compressive pressure is defined to be negative.

For a homogeneous and isotropic porous medium, the gas sorption-induced strain \(\varepsilon_s\) is presumed to result in volumetric strain only (Cao et al. 2016). The effects for the three normal components of strain are the same. A Langmuir-type equation is used to calculate
\( \varepsilon_s: \)
\[
\varepsilon_s = \frac{\varepsilon_L p}{P_L + p}
\] (5.5)

where \( \varepsilon_L \) is a constant representing the maximum volumetric strain for porous media and \( P_L \) is the Langmuir pressure constant.

From Equation (5.3), the volumetric strain is given as:
\[
\varepsilon_v = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = -\frac{1}{K} (\bar{\sigma} - \alpha p) + \varepsilon_s
\] (5.6)

where \( \bar{\sigma} = -\sigma_{kk}/3 \) represents the mean compressive stress and \( \sigma_{kk} = \sigma_{11} + \sigma_{22} + \sigma_{33} \).

Using the definition of porosity, the porosity change of a deforming shale formation can be expressed as (Cui and Bustin 2005):
\[
\Delta \phi = \phi \left( \frac{1}{K} - \frac{1}{K_p} \right) (\Delta \bar{\sigma} - \Delta p)
\] (5.7)

where \( K_p \) denotes bulk modulus of pores. If assuming constant \( K \) and \( K_p \), Equation (5.7) can be integrated with time to get:
\[
\frac{\phi}{\phi_0} = \exp \left[ \left( \frac{1}{K} - \frac{1}{K_p} \right) (\Delta \bar{\sigma} - \Delta p) \right]
\] (5.8)

where the subscript 0 refers to the initial state. Equation (5.8) is usually used to describe the porosity of shale gas reservoirs (Cao et al. 2016). The mean compressive stress can be obtained from:
\[
\bar{\sigma} - p = -K \left( \varepsilon_v + \frac{p}{K_s} - \varepsilon_s \right)
\] (5.9)

As the bulk modulus \( K \) is commonly several orders of magnitude larger than the pore volume modulus \( K_p \), it is reasonable to assume that:
\[
\frac{1}{K} - \frac{1}{K_p} \approx -\frac{1}{K_p}
\] (5.10)
Define the compressibility \(c_t = \frac{1}{K_p}\), which is obtained from the McKee’s model:

\[
c_t = c_{t0} \frac{1 - e^{-\alpha_0(\Delta \bar{\sigma} - \Delta p)}}{\alpha_0 (\Delta \bar{\sigma} - \Delta p)}
\]  

(5.11)

We implement an other porosity model herein which is general and can avoid any restriction on stress and strain condition imposed in practical applications (Charoenuppapanimit et al. 2014; Wei et al. 2016). Through the Betti-Maxwell reciprocal theorem, we can obtain:

\[
K_p = \frac{\phi}{\alpha} K
\]  

(5.12)

Substituting Equation (5.12) into (5.7) yields:

\[
\phi - \phi_0 = \phi \left( 1 - \frac{\alpha}{\phi} \right) \frac{\Delta \bar{\sigma} - \Delta p}{K}
\]  

(5.13)

Generally \((\Delta \bar{\sigma} - \Delta p)/K \ll 1\), and thus the equation can be simplified into:

\[
\frac{\phi}{\phi_0} = 1 - \frac{\alpha}{\phi_0} \frac{\Delta \bar{\sigma} - \Delta p}{K} = 1 + \frac{\alpha}{\phi_0} \Delta \varepsilon_{et}
\]  

(5.14)

where \(\Delta \varepsilon_{et} = -(\Delta \bar{\sigma} - \Delta p)/K\) is defined as the total effective volumetric strain. From Equation (5.9) we can obtain:

\[
\Delta \varepsilon_v = \Delta \varepsilon_{et} - \frac{\Delta p}{K_s} + \Delta \varepsilon_s
\]  

(5.15)

The following formulation is widely applied for the change of intrinsic permeability \(k_\infty\) with respect to porosity in shale gas reservoirs:

\[
\frac{k_\infty}{k_{\infty 0}} = \left( \frac{\phi}{\phi_0} \right)^3
\]  

(5.16)
5.1.3 **Apparent permeability**

The Knudsen number for determining the apparent gas permeability is:

\[ K_n = \frac{\lambda}{r_e} \]  

(5.17)

where \( \lambda \) is the mean free path of gas molecule, and the expression under real-gas condition is given by (Villazon et al. 2011):

\[ \lambda = \frac{k_B T Z}{\sqrt{2} \pi d_m^2 m} \]  

(5.18)

where \( T \) is temperature; \( Z \) is gas compressibility factor; \( d_m \) is gas molecule diameter; \( k_B = R/N_A \) is the Boltzmann constant; \( N_A \) is the Avogadro’s constant and \( R \) is the gas constant.

Adsorption layer thickness reduces the average pore radius and thus intrinsic permeability. The effective radius of the flow paths is updated as:

\[ r_e = r - d_{ads} \]  

(5.19)

Important parameters of porous media such as intrinsic permeability, porosity and tortuosity are required to calculate the mean hydraulic radius \( r \):

\[ r = 2\sqrt{2\tau} \sqrt{\frac{k_\infty}{\phi}} \]  

(5.20)

where \( \tau \) is tortuosity. From Equations (5.16) and (5.20), the average pore radius of the deformed shale can also be related to the porosity:

\[ \frac{r}{r_0} = \frac{\phi}{\phi_0} = 1 + \frac{\alpha}{\phi_0} \Delta \varepsilon_{et} \]  

(5.21)

The thickness of the gas-adsorption monolayer is interpolated on the basis of a Langmuir-type functional relationship (Jiang and Younis 2015):

\[ d_{ads} = d_m \frac{p}{p + P_L} \]  

(5.22)
We employ the apparent permeability model proposed by Florence et al. (2007) to characterize the non-Darcy gas flow in shale formation. Florence et al. (2007) extended the derivation of Karniadakis and Beskok (2001) to the following form that relies only on the Knudsen number $K_n$, and the effective intrinsic permeability:

$$k_a = k_{∞eff}(K_n) = k_{∞eff}(1 + α_K K_n) \left(1 + \frac{4K_n}{1 + K_n}\right)$$  \hspace{0.5cm} (5.23)

where $α_K$ is the rarefaction parameter:

$$α_K = \frac{128}{15\pi^2} \tan^{-1}(4^{0.4}K_n^0)$$  \hspace{0.5cm} (5.24)

Considering the effects of matrix compaction and adsorbed layer on the nanopore geometry, the effective intrinsic permeability is given as:

$$k_{∞eff} = \frac{r_e^2 \phi}{8 \tau}$$  \hspace{0.5cm} (5.25)

The generalized formulation that incorporates the overall contributions from effective stress, adsorption and flow regimes for the apparent gas permeability is (Huang and Ghassemi 2015; Cao et al. 2016):

$$k_a = \frac{(r - d_{ads})^2 \phi}{8} \left(1 + \frac{4K_n}{1 + K_n}\right)$$  \hspace{0.5cm} (5.26)

### 5.2 Mathematical models

Now present the mathematical models that describe the flow and mechanical behavior of a fractured porous medium. The physical domain $Ω$ is separated into two regions: the porous matrix and fracture, as shown in Figure 5.1. The external contour is defined by $Γ$, and the fracture surfaces are defined by $Γ_f$.

#### 5.2.1 Porous matrix

Two sets of equations are derived to include the gas flow mechanisms, mechanical
responses of shale matrix and their interactions. The mass conservation equation for a compressible single-phase fluid is:

\[
\frac{\partial}{\partial t} \left[ \phi \rho_g + (1 - \phi)m_g \right] = \nabla \cdot \left[ \rho_g \frac{k_a}{\mu} \nabla p \right] + q^W + q^{fm} \tag{5.27}
\]

where \( \rho_g \) is gas molar density; \( \mu \) is viscosity; \( q^W \) is the well sink term; \( q^{fm} \) denotes the mass communication between fracture and matrix, and has the similar expression as flux term; \( m_g \) is the molar mass of gas adsorbed in unit formation volume. We consider gas adsorption described by Langmuir isotherm in the accumulation term, and use the adsorption modified apparent permeability in the flux term to account for gas slippage and diffusion under the effect of volume reduction by the adsorbed layer.

We describe gas properties with real-gas option (density and viscosity). The model derived by Lee et al. (1966) is used for calculating gas viscosity. The gas molar density is computed as a function of pressure at isothermal conditions using the Peng-Robinson equation of state (PR-EOS):

\[
\rho_g = \frac{p}{RTZ} \tag{5.28}
\]

The shale deformation due to pressure change will affect the stress distribution and it will cause the change of average pore radius and intrinsic permeability. The quasi-static
momentum conservation equation for the solid skeleton and pore fluid is:

$$\nabla \cdot \sigma + \rho g = 0 \quad (5.29)$$

where \( \rho \) is the overall mass density; the symmetric total-stress tensor \( \sigma \) contains the contributions of both the fluid and the solid skeleton; \( \varepsilon \) is the strain tensor, which is linked with the displacement vector \( u \) through the kinematics relations:

$$\varepsilon = \nabla_s u \quad (5.30)$$

where \( \nabla_s \) is the symmetric gradient operator. The linear constitutive law without the sorption-induced strain can be given by:

$$\sigma' = D\varepsilon = D\nabla_s u \quad (5.31)$$

where \( D \) is the stiffness matrix. \( \Gamma_u \) and \( \Gamma_t \), shown in Figure 5.1, represent the Dirichlet and Neumann parts, respectively of the external boundary of the reservoir domain \( \Omega \).

5.2.2 Fracture

During gas production from shale reservoir, coupled gas flow and matrix deformation will cause the changes in fracture aperture and thus the fracture permeability (Ren et al. 2016). The stress-dependence of fracture will simultaneously influence the fluid flows in the whole reservoir, especially for long term production.

The discrete fractures are treated as lower dimensional objects \( (\mathbb{R}^{d-1}) \) with two surfaces \( (\Gamma_f^+ \) in a reservoir domain \( \Omega \in \mathbb{R}^d \), \( d = 2 \text{ or } 3 \). Equation (5.27) is also applicable as the governing equation for fracture, with slight difference that we neglect adsorption and apparent permeability. The displacement field across a fracture is discontinuous, while its gradient, the stress field, is continuous. The resulting jump in displacements \( w \) (fracture
aperture):

\[ w = \mathbf{n} \cdot (\mathbf{u}^+ - \mathbf{u}^-) \]  \hspace{1cm} (5.32)

where \( \mathbf{n} \) is the unit outward normal vectors; \( \mathbf{u}^+ \) and \( \mathbf{u}^- \) are displacements on the fracture upper and lower faces, respectively. Here we only consider the normal component of the displacements across fracture. The fracture permeability is usually given by:

\[ k_f = \frac{w^2}{12} \]  \hspace{1cm} (5.33)

For a fracture in equilibrium, force is not only transferred through the fluid, but also through the solid-solid contacts resulted from the proppants between the two surfaces. During the developments of shale gas reservoirs, it is very challenging to sustain sufficient fracture conductivity owing to the phenomena of proppant compaction, crushing or embedment. The reduction in fracture aperture as a function of pressure drawdown could have a significant impact on gas recovery. When proppants are present, deformed proppants will exert forces on the inner fracture faces and resist closure.

The total tractions acting on the opposite sides of a fracture are:

\[ t_N = p_f + t_p \]  \hspace{1cm} (5.34)

where \( p_f \) is the average fluid pressure inside fracture and \( t_p \) is the average pressure caused by proppants. Note that proppants are only effective when a fracture aperture is less than the initial width of the proppant. In case that the two surfaces lose physical contact, the surfaces are kept apart only by the fluid pressure, and thus \( t_p = 0 \). This implies that there is no contact force between the fracture faces. The total tractions have to satisfy the continuity conditions:

\[ t_N^+ = -t_N^- = t_N = t_N \mathbf{n} \]  \hspace{1cm} (5.35)
Finally the mechanics boundary conditions for the whole reservoir domain are given by:

\[
\begin{align*}
\mathbf{u} &= 0 \quad \text{on } \Gamma_u \\
\mathbf{\sigma} \cdot \mathbf{n} &= \mathbf{f} \quad \text{on } \Gamma_t \\
\mathbf{\sigma} \cdot \mathbf{n} &= \mathbf{t}_N \quad \text{on } \Gamma_f^\pm 
\end{align*}
\] (5.36)

5.2.3 Proppant-Fracture contacts

During well depletion, fracture conductivity may exhibit a significant loss due to the changes in formation stress state (Zhang et al. 2013). In relatively soft shale formations, the conductivity loss is attributed to the embedment of proppant particles into the shale rock (Zhang et al. 2015). It has been shown that the proppant embedment can be considerable and the proppant would fully embed in the soft shale (Chen et al. 2017). For hard formations, excessive deformation or crushing of proppant particles will be the mechanism that causes the fracture closure.

The proppant-fracture interactions are essentially the contact behavior of two non-conforming objects, which is a classic problem in the mechanics of materials and can be properly characterized using the contact mechanics models. Numerous analytical, experimental and numerical studies have been performed in the past in order to simulate and predict the contact properties, such as the real radius of contact, average pressure (i.e. hardness) and contact force (Ghaednia et al. 2016). The contact between a sphere and a flat is a fundamental aspect in contact mechanics and the normal force-displacement (NFD) relation is an important property for understanding the contact responses. For small deformation of linear elastic materials, the well-known Hertz theory (Hertz 1882) can effectively describe the NFD relation. However, the theory cannot be directly extended to describe large deformation associated with the plastic behavior. When the contact force reaches a critical value, the stress state will start to cause yielding within the objects (Jackson and Green 2005). Because of its complexity, the solution to the elasto-plastic contact problem mostly rely on the empirical formulations derived from numerical studies (i.e. FEM analysis).

Sphere-flat contact models are mainly divided into two types: the flattening and
indentation models. In the flattening models, the flat is considered to be rigid and the sphere is deforming, while for indentation the flat is deforming and the sphere is either rigid or elastic (Ghaednia et al. 2015). We can see that the flattening models are suitable for proppant compaction and crushing, while the indentation models for proppant embedment. In this work we implement two elasto-plastic contact models to characterize the complex interactions of proppant and fracture.

**Flattening case.**

Figure 5.2 shows an elasto-plastic sphere that is loaded against a rigid flat. \( \delta \) is the displacement of the tip of the contact point in the normal direction and \( a \) is the real radius of contact. Jackson and Green (2005) developed an empirical formulation (JG model) based on FEM results. They provided equations for the prediction of initial yielding in the sphere according to the von Mises yield criteria. The hardness is not considered to be constant for this model, and it is allowed to vary during the contact.

\[
F = \frac{4}{3} E' R^{\frac{3}{2}} \delta^2
\]  

(5.37)

where \( R \) is the radius of the proppant sphere; \( E' \) is the reduced modulus of elasticity, which considers the elastic properties of the two different materials in contact:

\[
\frac{1}{E'} = \frac{1 - \nu_p^2}{E_p} + \frac{1 - \nu_{sf}^2}{E_{sf}}
\]  

(5.38)
where $\nu_p$ and $\nu_f$ are the Poisson ratios of the proppant and shale, respectively; $E_p$ and $E_f$ are the moduli of elasticity.

$\delta_y$ is the critical displacement between the elastic and elasto-plastic phases:

$$\delta_y = \left( \frac{\pi C S_y}{2E'} \right)^2 R$$  \hspace{1cm} (5.39)

$\delta_y$ is the displacement at which yield starts and is derived from the von Mises yield criterion; $S_y$ is the yield strength of the weaker material, which in the flattening case is the proppant; and $C = 1.295 \exp(0.736\nu_p)$.

Now define a dimensionless displacement:

$$\delta^* = \frac{\delta}{\delta_y}$$  \hspace{1cm} (5.40)

In JG model the elasto-plastic phase effectively begins with $\delta^* = 1.9$ and the force is expressed as (Ghaednia et al. 2015):

$$F_{ep} = F_y \left[ e^{-0.17\delta^*/12} \delta^*^{1.5} + \frac{4HG}{CS_y} \left( 1 - e^{-\frac{4}{\pi}\delta^*/9} \right) \delta^*^{1.1} \right]$$  \hspace{1cm} (5.41)

where $F_y$ is the contact force when the yielding initiates; the average pressure to yield strength ratio is given as:

$$\frac{HG}{S_y} = 2.84 - 0.92 \left[ 1 - \cos \left( \frac{\pi a}{R} \right) \right]$$  \hspace{1cm} (5.42)

where,

$$a = \sqrt{R\delta^*(1.9)^B}, \quad B = 0.14 \exp(23S_y/E')$$  \hspace{1cm} (5.43)

The equation captures the effect that large deformations of the sphere have on the contact pressure. For the deforming sphere, the original curved contact morphs towards a cylindrical column in contact with a flat.

**Indentation case.**
In the indentation models which are suitable for describing proppant embedment, the contact between a deformable sphere and flat is shown in Figure 5.3. Ma and Liu (2015) develop an indentation model (ML model) with the $C^1$ continuity. The contact is divided into three phases: the elastic, mixed elastic-plastic, and fully plastic phase. Within the elastic phase, the force-displacement relation is also established via Hertzian theory. This stage ends when the pressure distribution on the contact surface reaches a threshold $p_y$, corresponding to a state where yielding initially occurs beneath the contact surface. As pressure exceeds $p_y$, a plastic deformation region is formed beneath the contact surface, and it enlarges as load increases. When the pressure distribution becomes approximately uniform and remains nearly constant, the contact state is in a fully plastic phase, during which the contact force linearly depends on the indentation. In ML model, interpolations are employed to guarantee the higher order continuity of the force-displacement curve.

The subscripts $(\cdot)_y$ and $(\cdot)_p$ are used to represent the variables at the end of the elastic regime and the onset of the fully plastic regime, respectively. ML model can be summarized as:

$$F(\delta) = \begin{cases} 
\frac{4}{3}E'R^\frac{1}{2}\delta^2 & \text{if } \delta < \delta_y \\
\delta (c_1 + c_2 \ln(\delta/\delta_y)) + c_3 & \text{if } \delta_y \leq \delta < \delta_p \\
F_p + k_1 (\delta - \delta_p) & \text{if } \delta \geq \delta_p
\end{cases} \quad (5.44)$$

where the parameters that are derived from the conditions for enforcing the property of $C^1$
where \( \psi \) and \( \xi \) are the dimensionless parameters. When the von Mises yield criteria are used to distinguish material plasticity, Hertz’s theory predicts that the elastic regime ends when \( p_y = 1.6 S_y \). \( S_y \) is the yield strength of the shale rock. The critical yielding displacement \( \delta_y \) is:

\[
\delta_y = \frac{\pi^2 R^2}{4E'2p_y^2}
\]  

(5.51)

The mixed elastic-plastic stage starts from \( \delta = \delta_y \) and ends at \( \delta = \delta_p \). The critical displacement \( \delta_p \) is:

\[
\delta_p = \xi^2 \delta_y / 2
\]  

(5.52)

Note that the \( C^1 \) continuities in ML model are favorable for the iterative solution technique that is based on Newton-type method.

We assume that proppants uniformly distributed as a monolayer inside fracture. Now
the average pressure caused by proppants on fracture inner faces can be calculated as:

\[ t_p = c_p \frac{F(\delta)}{\pi R^2} \]  

(5.53)

where \( c_p \) is the proppant concentration inside fracture; the displacement \( \delta \) for the contact mechanics models is related to fracture aperture as:

\[ \delta = 0.5 (w_{pi} - w) \]  

(5.54)

where \( w_{pi} \) is the initial width of proppant particles.

5.3 Discretization and solution schemes

Mimetic finite difference (MFD) is applied to approximate the fluid velocity. We employ the fracture cross flow equilibrium (FCFE) method (Hoteit and Firoozabadi 2008) to treat the fracture-matrix transfer in the lower-dimensional DFM model. The grid and computational domain for flow are shown in Figure 5.4. The finite-element discretization for mechanics will be presented in this section. The formulation leads to a set of coupled nonlinear algebraic equations, which are solved using a fully implicit temporal scheme.

5.3.1 Grid structure

The DFM model based on a conformal unstructured grid is used to explicitly repre-
sent the discrete fractures. A fracture is treated as an interface element between the two neighboring matrix cells. The conformal grid is employed to solve both the flow and mechanics problems. For flow, the MFD method is used to approximate the cell-centered and face pressures \( p \). For mechanics, the displacement unknowns \( \mathbf{u} \) are associated with the nodes of the matrix elements. A splitting-node technique is used such that each node along the fracture interface is assigned to double nodes, each with its own degrees of freedom but share the same coordinates (Levonyan 2011). The technique allows us to deal with the fracture interface conditions, which are determined from the nonlinear proppant-fracture contact models. The traction vectors \( \mathbf{t}_N \) are defined on each fracture segment, and their locations correspond to the face midpoint used for numerical integration. The splitting-node approach is also called the ‘zero-thickness interface element’ and is widely applied in the fracture mechanics literature (Barani et al. 2011; Khoei et al. 2011). The schematic of the computational domain for mechanics is shown in Figure 5.5.

5.3.2 Finite element method for pore- and fracture mechanics

Galerkin finite element method is used to discretize the mechanics problem. Standard linear triangular elements are employed, and pressure is constant within the elements. Multiplying Equation (5.29) by an arbitrary function, \( \delta \mathbf{u} \), such that \( \delta \mathbf{u} = 0 \) on \( \Gamma_u \) and integrating over the domain, we can derive the weak form of the mechanics equilibrium equation.
Through some manipulations, the weak formulation can be expressed as:

\[
\int_{\Omega} (\nabla_s \delta u)^T D \nabla_s u \, d\Omega - \int_{\Omega} (\nabla_s \delta u)^T (\alpha p + K \varepsilon_s) \, m \, d\Omega = \int_{\Omega} (\delta u)^T \rho g \, d\Omega + \int_{\Gamma_t} (\delta u)^T \bar{t} \, d\Gamma + \int_{\Gamma_f} (\delta w)^T \mathbf{t}_N \, d\Gamma
\]

(5.55)

where \( m \) is the vector form of Kronecker’s delta, \( m = [1, 1, 1, 0, 0, 0]^T \); \( w \) is crack opening displacement (Garipov et al. 2016):

\[
w = n \cdot (u^+ - u^-) \quad (5.56)
\]

In finite element method, the displacement unknowns are approximated using the values at a finite number of nodal points. This involves generating elements for the whole space and choosing the interpolation functions to express \( u \) with each element:

\[
u = N \tilde{u}, \quad \delta u = N \delta \tilde{u} \quad (5.57)
\]

where \( \tilde{u} \) is the vector of the nodal displacement; \( \delta \tilde{u} \) is the weighting function and \( N \) the conventional shape functions. Applying the Galerkin method, the vector form of the coupled discretized system for mechanics becomes:

\[
K \tilde{u} - Q - f = 0 \quad (5.58)
\]

where,

\[
K = \int_{\Omega} (\nabla_s N)^T D \nabla_s N \, d\Omega \\
Q = \int_{\Omega} (\nabla_s N)^T (\alpha p + K \varepsilon_s) \, m \, d\Omega \\
f = \int_{\Omega} N^T \rho g \, d\Omega + \int_{\Gamma_t} N^T \bar{t} \, d\Gamma + \int_{\Gamma_f} N^T \mathbf{t}_N \, d\Gamma
\]

(5.59)

After applying the Gaussian quadrature rule, a local linear system for each element \( \Omega^E \) can be obtained. Summation of local equations give rise to the global linear system.
5.4 Validation

The developed numerical code is validated against an analytical solution of Mandel’s problem. Abousleiman et al. (1996) presented a canonical example of nonmonotonic behavior in pore pressure following undrained loading. A rectangular plate of length $2a$ and width $2b$ is sandwiched between two rigid, impermeable plates. A constant compressive force $F$ is applied at the top and bottom of the plate. $F$ is the force per unit length in the $z$ direction. The fluid pressure is constant at the left and right boundaries, and fluid can be expelled from the domain. Because of the symmetry in the domain, only one quarter of the plate is analyzed.

Figure [5.6] shows the pressure distribution along the $x$ axis with time. The pressure in the plate interior first builds up at early time before the entire domain starts to deplete. The numerical solution gives results in agreement with the analytical solution.

![Mandel's Problem](image.png)

Figure 5.6: Mandel’s problem validation

5.5 Results

A 2D synthetic model is generated to contain a single-stage hydraulically-fractured horizontal well at the center of a reservoir with a stimulated fracture network. The hydraulic fractures are assumed to fully penetrate the formation. High-resolution is needed to accurately capture large pressure gradient near fracture. Therefore instead of using a
dual-continuum type of model, the stimulated fracture network is explicitly described as the discrete representations. The meshing technique employed for the DFM model is able to yield desirable local grid refinement (LGR) feature around fracture.

A constant compressive stress equal to 30E6 Pa is applied on the top and right edges of the domain. The displacements at the left and bottom edges are constrained in the horizontal and vertical directions, respectively. The parameters of the base model are summarized in Table 5.1. Note that the initial values for permeabilities, porosities and proppant width are defined before initialization of the geomechanics problem. Here we assume that shale rock is the weaker material, and thus only proppant embedment scenario is considered. The contact mechanics model for indentation is used to characterize the complex interactions between proppant and fracture. The normal force-displacement (NFD) relations for the base model with different elasto-plastic properties of shale rock are plotted in Figure 5.7. From the results we can see that the elasto-plastic properties have large impacts on the resistant forces responded to fracture closure.

![Figure 5.7: Force-displacement relations for proppant embedment (indentation contact)](image)

Sensitivity studies are conducted to investigate which factors have large impacts on well performance and ultimate recovery of shale gas formations. Different cases are examined and only one mechanism is turned off so that the effect of that mechanism can be clearly
Table 5.1: Specification of the synthetic base model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>LX LY</td>
<td>100 / 100</td>
<td>m</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>1</td>
<td>m</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>20E6</td>
<td>Pa</td>
</tr>
<tr>
<td>Initial matrix permeability</td>
<td>5E-20</td>
<td>m²</td>
</tr>
<tr>
<td>Initial fracture permeability</td>
<td>1E-12</td>
<td>m²</td>
</tr>
<tr>
<td>Tortuosity of shale matrix</td>
<td>2.714</td>
<td></td>
</tr>
<tr>
<td>Initial matrix porosity</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>Young’s modulus of shale (E)</td>
<td>1E9</td>
<td>Pa</td>
</tr>
<tr>
<td>Young’s modulus of solid constituent</td>
<td>1E10</td>
<td>Pa</td>
</tr>
<tr>
<td>Possion’s ratio of shale</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>Gas molecule diameter</td>
<td>0.7E-9</td>
<td>m</td>
</tr>
<tr>
<td>Langmuir volumetric strain constant</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Langmuir volume of CH₄</td>
<td>0.018</td>
<td>m³/kg</td>
</tr>
<tr>
<td>Langmuir pressure of CH₄</td>
<td>4E6</td>
<td>Pa</td>
</tr>
<tr>
<td>Rock bulk density</td>
<td>2500</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>343.15</td>
<td>K</td>
</tr>
<tr>
<td>Initial proppant width</td>
<td>0.005</td>
<td>m</td>
</tr>
<tr>
<td>Young’s modulus of proppant</td>
<td>6E10</td>
<td>Pa</td>
</tr>
<tr>
<td>Possion’s ratio of proppant</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>ψ of proppant</td>
<td>2.8</td>
<td></td>
</tr>
<tr>
<td>ξ of proppant</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td>Proppant concentration</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Yield strength of shale (Sᵧ)</td>
<td>500E6</td>
<td>Pa</td>
</tr>
<tr>
<td>Wellbore radius</td>
<td>0.1</td>
<td>m</td>
</tr>
<tr>
<td>Production BHP</td>
<td>6E6</td>
<td>Pa</td>
</tr>
<tr>
<td>Total simulation time</td>
<td>1200</td>
<td>day</td>
</tr>
</tbody>
</table>

The fracture geometry and pressure profile at the end of simulation for the base case are shown in Figure 5.8. The displacement magnitudes in the x direction Uₓ, in the y direction Uᵧ, and the displacement vector at the solution nodes U are shown in Figures 5.9, 5.10 and 5.11, respectively. The displacement profiles demonstrate that the developed mechanics model for discrete fracture can capture the discontinuities across the fracture faces.

The gas rates without considering the effects of different gas storage and flow mechanisms are shown in Figure 5.12. It is well-known that release of adsorption gas can compensate for pressure loss to some degree, and thus more gas can be produced at the
Table 5.2: Specification of the simulation cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Base case</td>
</tr>
<tr>
<td>2</td>
<td>Without sorption</td>
</tr>
<tr>
<td>3</td>
<td>Without the effect of adsorbed layer</td>
</tr>
<tr>
<td>4</td>
<td>Without the effect of apparent permeability</td>
</tr>
<tr>
<td>5</td>
<td>With sorption induced strain</td>
</tr>
<tr>
<td>6</td>
<td>Without variation from the initial sorption induced strain</td>
</tr>
<tr>
<td>7</td>
<td>Without the stress-dependent effects on matrix porosity and permeability</td>
</tr>
<tr>
<td>8</td>
<td>Without the stress-dependent effect on fracture permeability</td>
</tr>
</tbody>
</table>

Figure 5.8: Fracture geometry and pressure profile at the end of simulation

same pressure level. However the results show that the gas rate is even higher for CASE-2 (without sorption). This is because the effects of gas adsorbed layer and desorption are opposite, and the pore-radius reduction due to adsorbed layer has larger impact on gas rate. It also can be observed that the apparent permeability enhancement leads to higher gas rate.

Figure 5.13 shows the geomechanics effects on gas rate. In CASE-5 we consider gas sorption-induced strain with the Langmuir volumetric strain constant $\varepsilon_L = 0.05$, and $\varepsilon_s$ remains constant as its initial value in CASE-6. The sorption-induced strain plays an important role in the variations of shale porosity and permeability. From the results we can see that the adsorption induced swelling can compact the pores, leading to permeability decrease and thus reduction in gas rate. Comparing CASE-5 to CASE-6, it also can be
observed that matrix shrinkage due to desorption slightly improves the gas recovery in the late stage of production, indicating that matrix shrinkage results in permeability increase under the current mechanics boundary conditions. In addition, effective stress increases during gas depletion and it will compact the shale pores. CASE-7 shows that the stress-sensitive changes of matrix porosity and permeability strongly affect the well performance, especially for the late period. The result also clearly illustrates that the effect of formation compaction completely dominates the apparent permeability evolution for this simulation.
Figure 5.11: Displacement $U$

Figure 5.12: Effect of gas storage and flow mechanisms

scenario, in which the intrinsic permeability loss cannot be compensated by the non-Darcy flows including gas slippage and diffusion.

CASE-8 is performed without considering the stress-dependent fracture permeability. The simulated gas rate shows that fracture closure only causes an impact at the early depletion stage. This phenomenon is because of the extremely low permeability of shale matrix, which prevents the generation of an effective drainage region around hydraulic fractures.
Therefore maintaining high conductivity of fractures has limited effect on slowing down the gas rate decline. The explanation can be further supported by the cases with different elastic-plastic properties of shale rock in the proppant-fracture contact mechanics model. The results of gas rate are shown in Figure 5.14. The level of fracture closure depends on proppant embedment (indentation) which is controlled by the elastic-plastic properties. We can see from the figure that the cases have little differences on the gas rate, indicating that the overall influences of fracture conductivity are very limited. Under such a scenario, one reasonable way for boosting gas recovery is to create a denser and well-connected network of hydraulic fractures, instead of maintaining the conductivity of a single fracture. A denser fracture network can increase the contact area with the shale matrix and thus create a larger drainage region.

![Figure 5.13: Effect of geomechanics](image)

We perform another set of simulation studies on the base case with the initial matrix permeability changed to 1E-18 m$^2$. Again the effects of the elastic-plastic properties of shale rock are examined on the modified base case, and the gas rates are plotted in Figure 5.15. In this scenario, with a higher matrix permeability, the dynamic behavior of fracture closure can results in a larger impact on the late production stage. The fracture permeability loss
induced by proppant embedment is more significant for a weaker material strength of shale rock. It should be noted that in the case of proppant embedment, the fracture closure is mainly determined by the properties of shale rock, and thus cannot be offset simply through using a harder type of proppant particles.
Due to recent low gas prices, most of the operating companies have slowed down their activities in dry gas areas and refocused their attention on production from the gas-condensate window of liquid-rich regions (Fathi et al. 2013). The Eagle Ford, Barnett and Woodford shale in the U.S., and the Duvernay Shale in Canada are examples of liquid-rich shale (LRS) plays which are being exploited to produce more profitable liquid hydrocarbons with natural gas. However, this change in production plans requires detailed investigation of gas condensate bank development and saturation dynamics in the formation. An advanced level of understanding of the parameters and mechanisms affecting condensate recovery is necessary for achieving optimal development and operation plans. As the pressure in near-wellbore region drops below the dew-point, liquid droplets are formed and tend to be trapped in small pores; thus condensate blockage would occur and lead to a rapid decline in well productivity. It has been suggested that injection of CO$_2$ into shale gas reservoirs can be a feasible option to enhance recovery of natural gas and/or valuable condensate oil, while at the same time sequestering CO$_2$ underground (Godec et al. 2013; Eshkalak et al. 2014; Ren et al. 2015). Two methods are usually employed in the context of gas injection: gas flooding and huff-n-puff. Previous simulation studies showed that traditional well-to-well flooding for shale reservoirs might not be feasible because it is very difficult for the injected fluid to efficiently transport into the ultra-tight formation (Sanchez-Rivera et al. 2015). Therefore, it is advantageous to consider a cyclic huff-n-puff approach in which the same well alternates between injection and production. The injected CO$_2$ is expected to serve two purposes: 1) miscible interaction with the condensate phase to reduce the dew point pressure and to
improve oil mobility of the fluid system, and 2) repressurization of the reservoir so that pressure is raised above the dew point in near-wellbore region (Sheng 2015).

In order to achieve optimal development and operation plans for various enhanced oil recovery scenarios in shale gas reservoirs, there is considerable and timely interest in numerical simulation techniques which can accurately predict the complex production phenomenon. Unfortunately, existing simulation techniques fail to include the evolving understanding of the recovery physics associated with the fluid system that consists of multiple gas species or phases. Transport properties and mechanisms as well as phase behavior under nanoscale confinement exhibit deviations from their bulk behavior. Multiflow mechanisms such as slip flow, transition flow and Knudsen diffusion may co-exist, thus apparent permeability should be used to correct the flow deviation from the traditional Darcy’s law (Li et al. 2015). Desorption has also been suggested to be an important storage mechanism in organic-rich shales, particularly for heavy hydrocarbon fractions, which may contribute significantly to condensate production (Haghshenas et al. 2014). Moreover, molecular diffusion may take over as the main recovery mechanism under the severe effect of condensate bank impairment in fractured gas-condensate systems (Ayala et al. 2006).

Many studies indicate that the thermodynamic phase behavior of in-situ hydrocarbon mixtures in confined spaces significantly deviates from that of bulk fluids in the PVT cells (Wang et al. 2013; Jin et al. 2013; Alharthy et al. 2013; Teklu et al. 2014; Wang et al. 2014; Jin and Firoozabadi 2015; Rezaveisi et al. 2015; Xiong et al. 2015; Tan and Piri 2015). The nanopores in the ultra-tight shale formation could lead to significant interfacial curvature and capillary pressure between confined vapor and liquid phases. The work of Nojabaei et al. (2013) shows that without considering the effect of capillary pressure in vapor-liquid equilibrium (VLE) calculation a conventional reservoir simulator will likely not be able to explain the inconsistent produced gas-oil ratio (GOR) observed in the field compared to simulated results.

In this work, we develop a comprehensive compositional simulator for the modeling of gas-condensate shale reservoirs with complex fractured system. Related storage and

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transport mechanisms such as multicomponent apparent permeability (MAP), sorption and molecular diffusion are considered. Extended Langmuir model is implemented to simulate the multicomponent sorption behavior, and the ordinary diffusion flux driven by concentration gradient is considered in the form of Fick’s law. In order to accurately capture the complicated phase behavior of the multiphase fluids, an Equation of State (EOS) based phase package is incorporated into the simulator. The phase package takes into account the effect of the large capillary pressure that exists in ultra-tight shale matrix. A modified negative-flash algorithm that combines Newton’s method and successive substitution iteration (SSI) is used for phase stability analysis.

The developed simulator is used to understand and quantify the combined effect of capillary pressure and multicomponent mechanisms on the phase and production behavior in gas-condensate shale reservoirs. We present preliminary simulation studies to show the applicability of CO$_2$ huff-n-puff for the purpose of enhanced hydrocarbons recovery. Several design components such as the number of cycles and the length of injection period in the huff-and-puff process are also briefly investigated.

6.1 Gas-condensate systems

Gas-condensate reservoirs are characterized by the phase envelope of fluid system and the reservoir conditions. The phase envelope consists of the bubble-point line and the dew-point line meeting at the critical point as shown in Fig. 6.1 (Fan et al. 2005). If the reservoir temperature is between the critical temperature and the cricondentherm temperature, the reservoir will follow the path indicated by the black thick line during isothermal expansion. Retrograde condensation will start to occur at the reservoir when the variation path crosses the dew-point line.

As the pressure in the near-wellbore region drops below the dewpoint during production, liquid condensate droplets are formed and tend to be trapped in small pores or pore throats and not produce because of relative permeability effects. It was discovered that three regions with different liquid saturations emerge around a gas-condensate well producing be-
low the dewpoint pressure, as shown in Fig. 6.2. Away from the well, an outer region (3) contains the initial gas saturation. An intermediate region (2) shows a rapid condensate build-up and a corresponding reduction in gas relative permeability and thus the well productivity. Liquid in this region is still immobile because the critical saturation has not been reached yet. As a consequence, the produced gas contains fewer valuable heavy ends and the condensate that forms in most of the reservoir is lost to production. Nearer to the well, an inner region (1) forms where liquid saturation exceeds the critical saturation and both the reservoir gas and condensate are present and mobile.

6.2 Multicomponent storage and transport mechanisms

6.2.1 Apparent permeability

Unconventional gas formations are believed to be comprised of pores that are at the nano-scale, ranging in size from one to hundreds of nanometers. Conventional Darcy’s law does not adequately describe the various non-viscous gas flow regimes (e.g., slippage, transition and Knudsen diffusion) that may be present. As the length-scale of the pore throat diameter approaches the mean-free-path of the gas molecule, the continuum assumption does not apply (Javadvour et al. 2007). Such deviation has been proposed to be characterized
by the Knudsen number $K_n$,

$$K_n = \frac{\lambda}{R_h} \quad (6.1)$$

where $\lambda$ is the mean free path of gas molecule, and the expression under real-gas condition is given by (Michel et al. 2011),

$$\lambda = \frac{k_B T Z}{\sqrt{2\pi d_m^2 p_g}} \quad (6.2)$$

where $T$ is temperature; $Z$ is gas compressibility factor; $d_m$ is molecule diameter, $d_m = 10^{-10} \times 0.809 V_c^{1/3}$; $V_c$ is critical volume; $p_g$ is gas phase pressure; $k_B = R/N_A$ is the Boltzmann constant; $N_A$ is the Avogadro’s constant.

We can reformulate Eq. (6.2) through the following derivation,

$$\frac{p_g}{k_B T Z} = N_A \frac{p_g}{ZRT} = N_A \rho_g \quad (6.3)$$

where $\rho_g$ is gas molar density. And finally we get,

$$\lambda = \frac{1}{\sqrt{2\pi \rho_g N_A d_m^2}} \quad (6.4)$$
\( R_h \) is the mean hydraulic radius,

\[
R_h = 2\sqrt{2\tau_0} \sqrt{\frac{k_\infty}{\phi}} \tag{6.5}
\]

where \( \tau_0 \) is tortuosity, \( \phi \) is porosity, and \( k_\infty \) is the intrinsic permeability of porous media.

We implement the transport model proposed by Florence et al. (2007) in our numerical simulator. Florence et al. (2007) extended the derivation of Karniadakis et al. (2001) to the following form that relies only on the Knudsen number \( K_n \), and the Darcy permeability,

\[
k_a = k_\infty f(K_n) = k_\infty (1 + \alpha_K K_n) \left( 1 + \frac{4K_n}{1 + K_n} \right) \tag{6.6}
\]

where the term \( \alpha_K \) is the rarefaction parameter,

\[
\alpha_K = \frac{128}{15\pi^2} \tan^{-1}(4K_n^{0.4}) \tag{6.7}
\]

For the liquid-rich shale reservoirs, the apparent permeability correction for multicomponent mixture could be described by using a mean free path \( \lambda_i \) which differs for each species in the mixture. The apparent permeability correlation for component \( i \) is,

\[
k_{ai} = k_\infty f(K_{ni}) \tag{6.8}
\]

6.2.2 Sorption

Sorption process can play a key role in determining flow and composition of gas and condensate produced from organic-rich shale gas reservoirs. The adsorption capability of different hydrocarbon component is known to increase strongly with molecular weight. The laboratory data provided by Ambrose et al. (2011) illustrates that adsorption on organic matter may be an important storage mechanism for the heavy hydrocarbon fractions.

The extended Langmuir (EL) isotherm which describes the fractional surface coverage of each component is used here for describing the multicomponent sorption behavior (Yang
We choose to apply EL due to its simplicity and wide usage across the petroleum industry, although more advanced sorption model could be substituted in its place.

The molar quantity of adsorbed gaseous component can be expressed as,

\[ m_{gi} = \rho_R \rho_{gs} V_{gi} \] (6.9)

The standard volume of gaseous component \( i \) adsorbed per unit rock mass is,

\[ V_{gi} = \frac{V_{Li}(p_{gi}y_i)/P_{Li}}{1 + \sum (p_{gi}y_i/P_{Li})} \] (6.10)

where \( V_{Li} \) is the Langmuir volume of component \( i \) (the maximum adsorption capacity at a given temperature), and \( P_{Li} \) is the Langmuir pressure of component \( i \) (the pressure at which the adsorbed gas content is equal to \( V_{Li}/2 \)). \( \rho_R \) is the rock bulk density; \( \rho_{gs} \) is the gas molar density at standard condition; \( V_{gi} \) is the adsorption isotherm function.

6.2.3 Molecular diffusion

Molecular diffusion refers to the relative motion of different gas species and will cause the concentration gradients to gradually equilibrate (Freeman et al. 2011). Where processes such as Knudsen diffusion cause gas species to be separated, molecular diffusion will counteract any fractionating effects. Consequently, it is always necessary to include the gas diffusion term in any attempt to model Knudsen diffusion.

In addition, molecular diffusion may play an important role in the scenario of fractured gas-condensate shale reservoirs. After depletion in the fracture network, an undesirable coating of condensate surrounding the matrix blocks will form. If the matrix blocks are extremely tight, the inner portion of the matrix blocks may not “feel” the pressure change until a later depletion stage; thus most of the gas originally in place will be trapped and may not be easily recovered. This condensate bank impairment can be quite severe for systems with very low permeability, and molecular diffusion might take over as the primary mechanisms for fluid flow in conjunction with Darcian flow (Ayala et al. 2009).
In multicomponent mixtures, the classical Fick’s law assuming that each component diffuses as a result of its own concentration gradient is often used for modeling molecular diffusion. Gas diffusivity values are commonly adjusted to effective diffusion coefficient for porous media (Ho and Webb 2006),

$$D_e^i = \phi S_g \tau_0 \tau_g \rho_g D_{gi}$$  \hspace{1cm} (6.11)

where $D_{gi}$ is the diffusion coefficient of component $i$ in bulk gas; $\tau_0 \tau_g$ is the tortuosity which includes a porous medium dependent factor $\tau_0$ and a coefficient that depends on gas phase saturation $S_g$,

$$\tau_0 \tau_g = \phi^{1/3} S_g^{7/3}$$  \hspace{1cm} (6.12)

Liquid diffusion coefficients are usually orders of magnitude lower than gas phase diffusion coefficients at the same thermodynamic conditions; thus diffusive effect is not considered to make a significant contribution in liquid flows (Ayala et al. 2009; Freeman et al. 2011). We assume here that molecular diffusion only takes place in the gas phase, while the flow of the liquid phase is only attributable to pressure gradients.

6.2.4 Phase equilibrium calculations

The average pore size can be on the order of tens of nanometers for shale and tight-rock formations. Such small pores lead to significant interfacial curvature and capillary pressure between confined vapor and liquid phases. The thermodynamic phase behavior of in-situ hydrocarbon mixtures may be significantly different from that of bulk fluids in the PVT cells. Several studies show that the large capillary pressure has significant effect on the shift of phase envelope (Pang et al. 2013; Nojabaei et al. 2013; Nojabaei et al. 2014; Teklu et al. 2014). In this paper, we use PR-EOS coupled with the Young-Laplace equation, to perform the vapor-liquid equilibrium (VLE) calculation for the confined fluids in nanosize pores. The requirement of vapor-liquid equilibrium is the equality of phase chemical
potentials for each component $i$ in the fluid mixture of $n_c$ components:

$$\mu_i^v(y, T, p^V) = \mu_i^l(x, T, p^L), \quad i = 1, ..., n_c$$  \hspace{1cm} (6.13)

where $y = \{y_i\}$, $x = \{x_i\}$ are the mole fractions of component $i$ in the vapor and liquid phases. For practical use, the chemical potentials in Eq. (6.13) are usually related to fugacity $f$ as follows,

$$f_i^v(y, T, p^V) = f_i^l(x, T, p^L)$$  \hspace{1cm} (6.14)

$$y_i \Phi_i^{V,p^V} = x_i \Phi_i^{L,p^L}, \quad i = 1, ..., n_c$$

The fugacity coefficients $\Phi$ can be determined through an Equation of State (EOS), for example, Peng-Robinson (PR) EOS,

$$\ln \Phi_i = \frac{b_i}{Z - 1} - \ln (Z - B) - \frac{A}{2\sqrt{2}B} \left( \frac{1}{a_i} \frac{\partial a}{\partial x_i} - \frac{b_i}{b} \right) \ln \frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B}$$

$$\frac{\partial a}{\partial x_i} = 2 \sqrt{a_i} \sum_{j=1}^{n} x_j (1 - k_{ij}) \sqrt{a_j}$$  \hspace{1cm} (6.15)

Note that the fugacities are evaluated at the same temperature $T$ but at different phase pressures, which are related to each other through the capillary pressure $p_c$,

$$p^V = p^L + p_c$$  \hspace{1cm} (6.16)

Capillary pressure is calculated on the basis of the Young-Laplace equation in which the principle radii of curvature are equal,

$$p_c = \frac{2\sigma \cos \theta}{r}$$  \hspace{1cm} (6.17)

where $r$ is the average pore radius; $\sigma$ is interfacial tension (IFT); $\theta$ is the contact angle of the vapor-liquid interface with respect to the solid surface of porous medium. IFT changes
as a function of composition by the Macleod and Sugden correlation (Pedersen et al. 2014),

\[
\sigma^{1/4} = \sum_{i=1}^{n_c} P_i (x_i \rho_L - y_i \rho_V)
\] (6.18)

where \( P_i \) is the parachor of pure components = \((8.21307 + 1.97473 \omega_i) T_{ci}^{1.03406} p_{ci}^{-0.82636} \); \( \omega_i \) is the accentric factor; \( T_{ci} \) and \( p_{ci} \) are the critical temperature (\( K \)) and critical pressure (bar) of each component, respectively.

During the compositional simulation, a stability analysis routine is needed to detect phase disappearance/reappearance (phase-state identification) for each gridblock at every Newton step (Rezaveisi et al. 2015). This can be achieved by a standard negative flash procedure, in which successive substitution iteration (SSI) is employed to find an initial guess for the K-values, followed by Newton’s method to final convergence. Here we present a modified SSI algorithm to accommodate the effect of capillarity on VLE calculation. The algorithm is summarized as follows,

1. Make an initial guess for the equilibrium ratio \( K \) which can be computed from Wilson’s equation,

\[
K_i = \frac{y_i}{x_i} = \frac{p_{ci}}{p} \exp \left( 5.37 (1 + \omega_i) \left( 1 - \frac{T_{ci}}{T} \right) \right)
\] (6.19)

2. The mixture is then flashed in order to determine the vapor and liquid compositions.

The overall composition of component \( i \) can be expressed as,

\[
z_i = l x_i + (1 - l) y_i
\] (6.20)

where \( l \) is the mole fraction of the mixture that is present in liquid phase. We can derive the Rachford-Rice equation, which is solely a function of \( l \) for a given \( z_i \) and \( K_i \), by using the fact that the mole fractions in each phase must sum up to unity,

\[
0 = 1 - 1 = \sum_{i=1}^{n_c} y_i - \sum_{i=1}^{n_c} x_i = \sum_{i=1}^{n_c} (y_i - x_i) = \sum_{i=1}^{n_c} \frac{(K_i - 1) z_i}{l + (1 - l) K_i}
\] (6.21)
Solve for $l$ from Eq. (6.21) and then solve for $x_i$, $y_i$ from the following equations,

\[
\begin{align*}
x_i &= \frac{z_i}{l + (1 - l)K_i} \\
y_i &= \frac{K_i z_i}{l + (1 - l)K_i}
\end{align*}
\]  

(6.22)

3. Update capillary pressure through Eq. (6.17) and the corresponding phase pressures.

4. Calculate the compressibility factor $Z$ for each phase from an EOS. Then calculate the fugacity for each component in each phase.

5. Check convergence $\sum_{i=1}^{n_c} \left(1 - \frac{f^L_i}{f^V_i}\right)^2 < \varepsilon$.

6. If not converged, update $K_i = K_i \left(\frac{f^L_i}{f^V_i}\right)$, and repeat step 1 to 5.

In this study, we only focus on the effect of capillary pressure on the VLE calculation. For pores larger than 10 nm, fluid phases are homogeneous and surface adsorption can be neglected. For pores smaller than 10 nm, strong fluid/surface interactions result in a heterogeneous density distribution and surface adsorption becomes significant. According to Li et al. (2014) and Jin et al. (2015), the assumption of bulk-phase thermodynamics is no longer valid and other fluid models such as density functional theory and Monte Carlo simulations are needed for pores less than 10 nm.

It has been reported that organic-inorganic configuration exists in shale: tiny organic material (kerogen) is scattered through predominantly inorganic material (Ambrose et al. 2012; Sun et al. 2014). The organic material mainly consists of nanopores with a narrow pore size distribution of approximately 2 nm, while inorganic pores have much larger sizes. As was pointed out by Sun et al. (2014), the fluid travel time in the organic material region is far shorter compared with inorganic material because of small organic cluster size. Therefore in this work we assume that the rapid fluid transfer process from organic material can be neglected and the organic-inorganic dual-continuum system can be homogenized into a single-continuum matrix model, as shown in Fig. 6.3. It is also assumed that the inorganic matrix mainly consists of pore sizes larger than 10 nm; thus two phase equilibrium under
the effect of interface curvature is sufficient and the phase behavior can be described by bulk-phase thermodynamics (using conventional EOS). The mass contributions from the adsorbed and free phase in organic nanopores are treated together as a source term which feeds the inorganic pore system. The source feeding behavior is characterized by EL model or sorption data obtained from laboratory measurement. We do not intend to directly deal with the complicated adsorbed-vapor-liquid phase equilibriums in the organic nanopores under confinement.

Figure 6.3: Single-continuum matrix model homogenized from the organic-inorganic configuration

6.3 Governing equations and numerical approaches

6.3.1 Governing equations

The three-phase multicomponent flow model which assumes that there is no mass transfer between the hydrocarbon (oil and gas) and water phases is used in this work. The model assumes gas is stored in fracture as free phase, while in matrix as both free and adsorbed phase. In an isothermal system containing $n_c$ mass components, subject to gravity effect, molecular diffusion (only for gas phase) and adsorption, $(2 \times n_c + 6)$ equations are needed to fully describe the system (matrix or fracture) with vapor-liquid equilibrium. A general compositional model is derived based on mass conservation law. The governing equation for each mass component is,

$$\frac{\partial N_i}{\partial t} = F_i + q^{fm}_i + q^W_i$$

(6.23)
where subscript \(i\) is the index for mass component, \(i = 1, ..., n_c, n_w\) with \(n_c\) being the hydrocarbon components and \(n_w\) being the water component. \(N_i\) is the mass accumulation term; \(F_i\) is the mass flux term; \(q_i^W\) is the source/sink term; \(q_i^{fm}\) denotes the mass communication between fracture and matrix, and it has the similar expression as the flux term.

Accumulation term \(N_i\) which considers the gas adsorption can be evaluated as,

\[
N_i = \phi(S_o\rho_o x_i + S_g\rho_g y_i) + (1 - \phi)m_{gi}
\]  
(6.24)

where \(m_{gi}\) is the molar mass of gas component \(i\) adsorbed in unit formation volume, and \(i = 1, ..., n_c\) denoting hydrocarbon components. \(x_i\) and \(y_i\) is the component mole fraction in oil and gas phases, respectively. For water component,

\[
N_w = \phi S_w\rho_w
\]  
(6.25)

The flux term which includes the combined driving forces resulted from pressure and concentration gradients for hydrocarbon component \(i\) is,

\[
F_i = -\nabla \cdot (\rho_o x_i \mathbf{u}_o + \rho_g y_i \mathbf{u}_{gi}) + \nabla \cdot (D_i \nabla y_i)
\]  
(6.26)

For water component we have,

\[
F_w = -\nabla \cdot (\rho_w \mathbf{u}_w)
\]  
(6.27)

Darcy’s law is used for the phase velocity,

\[
\mathbf{u}_\beta = -\frac{k_{r\beta}}{\mu_\beta} (\nabla p_\beta - \gamma_\beta g \nabla D)
\]  
(6.28)

where \(\beta = o, g, w\). For the gas phase \(\mathbf{u}_g\) is dependent on \(i\) and \(k = k_{ai}\) (apparent permeability); For the other phases \(k = k_\infty\) (intrinsic permeability); \(k_{r\beta}\) is the phase relative permeability; \(\gamma_\beta\) is the phase mass density, \(kg/m^3\); \(\mu_\beta\) is the phase viscosity, \(Pa.s\).

Eq. (6.23) is applicable for different domains, with the slight difference that we neglect
adsorption and apparent permeability for fracture domain. In order to close the system, the saturation and capillary pressure constraints are needed,

\[ S_o + S_g + S_w = 1 \]
\[ p_{cgo} = p_g - p_o \]
\[ p_{cow} = p_o - p_w \]  \hspace{1cm} (6.29)

The fugacity constraints for thermodynamic equilibrium between oil and gas phases and the composition constraints are also needed,

\[ f^o_i - f^g_i = 0 \]
\[ \sum_{i=1}^{n_c} x_i = 1, \quad \sum_{i=1}^{n_c} y_i = 1 \]  \hspace{1cm} (6.30)

The fluid phase viscosities are computed through the correlation of Lohrenz et al. (1964). We employ two sets of capillary pressure and relative permeability curves for matrix and fracture. We assume that there is no capillary pressure inside fracture domain, and the capillary pressures in matrix domain are calculated from Eq. (6.17). A constant oil/water surface tension is assumed, and the gas/oil surface tension is calculated from Eq. (6.18). For fracture relative permeability, straight-line model is used. For matrix, it is usual to assume that relative permeability of wetting and non-wetting phases are the function of their saturations only, and relative permeability of an intermediate-wetting phase is a function of both saturations of wetting and non-wetting phase. For example, the three-phase oil relative permeability for a water wet system could be estimated using Aziz and Settari’s version of Stone’s equation (Aziz and Settari 1979),

\[ k_{ro} = k_{roiw} \left( \left( \frac{k_{row}}{k_{roiw}} + k_{rw} \right) \left( \frac{k_{rog}}{k_{roiw}} + k_{rg} \right) - (k_{rw} + k_{rg}) \right) \]  \hspace{1cm} (6.31)

Nagarajan et al. (2013) show that the wettability of shale formation is highly heterogeneous and can vary from condensate-wet to water-wet, with dominant mixed-wettability. The water-wet relative permeability assumed here can be replaced by other available alternatives.
6.3.2 Finite-volume discretization

The finite-volume formulation which is very flexible for handling interactions between various kinds of continua is applied for discretizing the governing equations. The two-point flux approximation (TPFA) is used to approximate the flux at the interface shared between two control volumes. We implement a lower-dimensional discrete fracture and matrix (DFM) model based on unstructured gridding to handle the complex fracture geometries of hydraulic fracture in stimulated formation. Optimized local grid refinement (LGR) is employed to accurately capture the transient flow regime around fractures. For the well term discretization of multifractured horizontal well, we assume that the reservoir fluids only flow from hydraulic fractures into the wellbore at perforated points, and there is no pressure drop along the horizontal wellbore.

6.4 Simulation results and discussions

A synthetic model is generated to contain a single-stage hydraulically-fractured horizontal well at the center of a reservoir with a stimulated fracture network. The hydraulic fractures are assumed to fully penetrate the formation. The model grid set up is shown in Fig. 6.4 and some basic model specifications appear in Table 6.1. The fracture conductivity is obtained from the value range recorded in Zhang et al. (2013; 2015). Here we take component diffusion coefficient to be equal to avoid violation of the total flux balance. The relative permeability and sorption data are summarized in Tables 6.2 and 6.3. A set of 7-component compositional model is generated based on PVT data published by Orangi et al. (2011). The reservoir fluid composition, Peng-Robinson EOS parameters and interaction coefficients for the gas-condensate system are presented in Tables 6.4 and 6.5.

Condensate dropout below the dew-point pressure can cause significant variation of fluid compositions and complicated flow behavior in both the fractures and matrix. High-resolution is needed to accurately capture large pressure gradient and condensate blockage near fracture (Fu et al. 2005; Sun and Schechter 2015; Sun et al. 2015). Therefore instead of using dual-continuum model, the stimulated fracture network is explicitly described as
Table 6.1: Basic model specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir dimensions (x, y)</td>
<td>160, 120</td>
<td>m</td>
</tr>
<tr>
<td>Formation thickness</td>
<td>10</td>
<td>m</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>23</td>
<td>MPa</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>480</td>
<td>K</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>Intrinsic matrix permeability</td>
<td>6e-20</td>
<td>m²</td>
</tr>
<tr>
<td>Rock density</td>
<td>2500</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Tortuosity</td>
<td>2.714</td>
<td></td>
</tr>
<tr>
<td>Fracture width</td>
<td>3e-3</td>
<td>m</td>
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<tr>
<td>Fracture permeability</td>
<td>1e-12</td>
<td>m²</td>
</tr>
<tr>
<td>Water viscosity</td>
<td>5e-4</td>
<td>Pa.s</td>
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<tr>
<td>Water compressibility</td>
<td>4.3946e-10</td>
<td>1/Pa</td>
</tr>
<tr>
<td>Contact angle θ</td>
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<td></td>
</tr>
<tr>
<td>Oil/water surface tension</td>
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<td>N/m</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>1e-7</td>
<td>m²/s</td>
</tr>
<tr>
<td>Well radius</td>
<td>0.1</td>
<td>m</td>
</tr>
<tr>
<td>Production BHP</td>
<td>8</td>
<td>MPa</td>
</tr>
<tr>
<td>Injection BHP</td>
<td>22</td>
<td>MPa</td>
</tr>
<tr>
<td>Production time</td>
<td>700</td>
<td>day</td>
</tr>
</tbody>
</table>

discrete representations. The meshing technique employed for the DFM model is able to yield desirable LGR feature around fracture.

Here we analyze the variation of the ratio $k_{ai}/k_{∞}$ with pressure for different compo-
Table 6.2: Relative permeability data

<table>
<thead>
<tr>
<th></th>
<th>$k_{roiw}$</th>
<th>$S_{gr}$</th>
<th>$e_{og}$</th>
<th>$e_{ow}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{rwro}$</td>
<td>1.0</td>
<td>0.0</td>
<td>2.0</td>
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<tr>
<td>$S_{org}$</td>
<td>0.2</td>
<td>0.1</td>
<td></td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 6.3: Sorption data

<table>
<thead>
<tr>
<th></th>
<th>CO2</th>
<th>C1</th>
<th>C2</th>
<th>IC4</th>
<th>C8</th>
<th>C11+</th>
<th>C15+</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_L$ (MPa)</td>
<td>2</td>
<td>5</td>
<td>3</td>
<td>2</td>
<td>1.8</td>
<td>1.8</td>
<td>1.8</td>
</tr>
<tr>
<td>$V_L$ ($m^3/kg$)</td>
<td>0.06</td>
<td>0.022</td>
<td>0.032</td>
<td>0.054</td>
<td>0.068</td>
<td>0.068</td>
<td>0.068</td>
</tr>
</tbody>
</table>

Table 6.4: Fluid system properties

<table>
<thead>
<tr>
<th>Component</th>
<th>Molar fraction</th>
<th>Critical pressure (bar)</th>
<th>Critical temperature (K)</th>
<th>Acentric factor</th>
<th>Molar weight</th>
<th>Critical volume ($m^3/kmol$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2</td>
<td>0.01</td>
<td>73.9</td>
<td>304.7</td>
<td>0.225</td>
<td>44.01</td>
<td>0.094</td>
</tr>
<tr>
<td>C1</td>
<td>0.72</td>
<td>46</td>
<td>190.6</td>
<td>0.013</td>
<td>16.04</td>
<td>0.098</td>
</tr>
<tr>
<td>C2</td>
<td>0.169</td>
<td>48.8</td>
<td>305.4</td>
<td>0.0986</td>
<td>30.07</td>
<td>0.148</td>
</tr>
<tr>
<td>IC4</td>
<td>0.042</td>
<td>36.5</td>
<td>408.1</td>
<td>0.1848</td>
<td>58.12</td>
<td>0.263</td>
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<tr>
<td>C8</td>
<td>0.037</td>
<td>28.8</td>
<td>575</td>
<td>0.312</td>
<td>107</td>
<td>0.433</td>
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<tr>
<td>C11+</td>
<td>0.0205</td>
<td>20.5</td>
<td>692.2</td>
<td>0.5491</td>
<td>175</td>
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<tr>
<td>C15+</td>
<td>0.0015</td>
<td>17.9</td>
<td>737.6</td>
<td>0.6435</td>
<td>210</td>
<td>0.841</td>
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Table 6.5: Interaction coefficients

<table>
<thead>
<tr>
<th></th>
<th>CO2</th>
<th>C1</th>
<th>C2</th>
<th>IC4</th>
<th>C8</th>
<th>C11+</th>
<th>C15+</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2</td>
<td>0</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.095</td>
<td>0.089</td>
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<tr>
<td>C1</td>
<td>0.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.037</td>
<td>0.051</td>
<td>0.062</td>
</tr>
<tr>
<td>C2</td>
<td>0.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.01</td>
<td>0.041</td>
<td>0.049</td>
</tr>
<tr>
<td>IC4</td>
<td>0.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C8</td>
<td>0.1</td>
<td>0.037</td>
<td>0.01</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C11+</td>
<td>0.095</td>
<td>0.051</td>
<td>0.041</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C15+</td>
<td>0.089</td>
<td>0.062</td>
<td>0.049</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

components based on the above model parameters. **Fig. 6.5** shows that lighter components will have larger flow capacity (higher apparent permeability ratio) because of smaller molecule diameter and then larger mean free path. The results illustrate that the multiple components effect should be captured by the MAP model instead of using a single pseudo-component apparent permeability.
We validate the developed phase package in our simulator against a commercial PVT simulation software (Calsep PVTsim 2013) as shown in Fig. 6.6. The phase envelopes under the bulk condition are compared and good agreement is obtained between the two simulated data. We also plot a part of phase envelope under the bulk condition and nanopore confinement with different intrinsic permeabilities which could be related to pore size through Eq. (6.5). Note that only the retrograde condensation region between the critical point and the cricondentherm is generated to clearly show the effect of capillary pressure. As we can see from Fig. 6.7 within the upper dew point branch the saturation pressure increases with smaller intrinsic permeability and the cricondentherm is also shifted towards a higher temperature. The greatly elevated dew point curve is expected to further exacerbate the productivity damage due to condensate bank development.

### 6.4.1 Effect of capillarity on phase behavior

When the fluid is confined in pore spaces of nanosize, the significant interfacial curvature may cause a large capillary pressure difference between liquid and vapor phases. We run simulation cases with and without considering capillary pressure (Pc) under the combined effect of previously mentioned multicomponent mechanisms, to investigate the corresponding impact on gas and condensate recovery. The pressure profiles at 100 and 700 day of the...
Figure 6.6: Validation for the phase envelope of the developed phase package against PVTsim

Figure 6.7: The upper dew point branch of phase envelope under the bulk condition and nanopore confinement

matrix grid for the case with Pc are shown in Fig. 6.8. The oil saturation profiles of the two cases at 700 day are also compared in Fig. 6.9. Figs. 6.11 and 6.12 show the gas and oil rates under the surface condition (1 bar, 25 °C) for the two cases. As can be seen, oil rate with the Pc effect (“all mechs” case) is much higher than the “no Pc” case, because
the elevated dew point pressure in the fluid system leads to more condensate dropout and thus higher oil saturation. In contrast, gas rate is lower under the effect of Pc due to the reduction in gas relative permeability caused by more significant condensate blockage. The results illustrate that the large capillary pressure has significant effects on phase behaviors, which cannot be ignored for reliable modeling of gas-condensate shale reservoirs.

During the early period of pressure depletion, a rapid condensate build-up in fractures and the surrounding matrix along with the boost in oil mobility is observed. This behavior leads to a rapid increase of oil rate, followed by a gradually declining process. We also plot the gas relative permeability profile at 100 day of the matrix grid for the “all mechs” case in Fig. 6.10. The figure indicates that a layer of condensate banking near fractures is formed and will result in permanent impairment to the gas productivity.

6.4.2 Effect of storage and transport mechanism

We study the effect of multicomponent storage and transport mechanisms on gas and condensate production. To isolate the effect of each mechanism, seven simulation cases are designed by turning specific mechanisms on or off, as shown in Table 6.6. We plot the cumulative gas and oil production (under the surface condition) for the first 5 cases in Figs. 6.13 and 6.14 and the other cases in Figs. 6.15 and 6.16. The oil saturation profiles at...
700 day for the cases 1/3/6/7 are shown in Figs. 6.17 and 6.18. We can see that Case 1 yields the highest cumulative gas production, and the effect of molecular diffusion makes little difference in the result under this simulation scenario. Although neglecting adsorption (Case 2) could lead to high gas rate in an early period due to less condensate dropout and thus smaller gas mobility reduction, the released gas contribution from adsorption will become more significant in the late period. Much less produced oil is observed in Case 2 and oil production becomes constant after a short period. This indicates that the oil saturation in matrix does not exceed the critical saturation limit and the oil phase becomes immobile. The results illustrate that desorption has large impact on well performance and could be an im-
important storage mechanism for heavy hydrocarbon fractions, which contributes significantly to condensate production.

Case 3 clearly shows the positive effect of MAP on gas flow capacity and thus well productivity. The result also shows an increase in oil production with considering MAP. This phenomenon could be explained by the fractioning effect of different hydrocarbon species in the flowing mixture. Lighter components have larger flow capacity and the valuable heavy
components will be left behind in the formation. Then faster condensate accumulation will lead to higher oil mobility and thus more oil production. However, it should be noted that this is just a relatively short-term behavior because under the effect of MAP, the valuable components are more likely to be lost during production and more difficult to be recovered from a long-term perspective. This mobility dominant mechanism could also be the reason why molecular diffusion exhibits the negative impact on oil recovery under the short-term production scenario set up in this paper.

Table 6.6: Model setting of the seven simulation cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Adsorption</th>
<th>MAP</th>
<th>Molecular diffusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 2</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 3</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 4</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 5</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 6</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Case 7</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

Figure 6.13: Cumulative gas production for the 5 cases

6.4.3 CO₂ huff-n-puff injection

During the primary depletion of a gas-condensate shale reservoir, condensate banking
can cause severe impairment to the well productivity. The appearance of condensate on the matrix-block faces will constrain gas withdrawal from the inner parts in the stimulated fracture network. The produced gas contains fewer valuable heavy ends and the dropout that forms in most of the reservoir will be lost to production. $CO_2$ huff-n-puff injection is a promising method to remove condensate blockage from the near wellbore region using miscible interactions between $CO_2$ and condensed liquid phase. The injected $CO_2$ is expected to re-pressurize the reservoir for boosting the driven energy, and to reduce the dewpoint pressure of the fluid system. Huff-n-puff cyclic injection scheme consists of three periods:
injection, soaking, and production. During the soaking period, well is shut-in to allow time for mass transfer between the injected $CO_2$ and condensate phase. Previous studies show that the soaking times have no benefits and are actually detrimental to production for unconventional shale reservoirs (Meng et al. 2015; Sheng et al. 2016).

We conduct preliminary simulation studies to examine the potential of $CO_2$ huff-n-puff for enhanced hydrocarbons recovery in gas-condensate shale reservoirs. No soaking time is added in the following simulation cases. The injection BHP is 22 $MPa$. The cyclic injection strategy with equal time (60/80/100/140 days) for the huff and puff periods is first compared with the depletion mode (base case). The gas rate and cumulative production of
hydrocarbon components under the surface condition (the produced CO$_2$ not included) are shown in Figs. 6.19 and 6.20 and the results for the oil phase are shown in Figs. 6.21 and 6.22. As can be seen, the gas recovery is improved a lot for CO$_2$ huff-n-puff scheme compared with the base case. Higher recovery is also observed for the cases with shorter cyclic interval, for the reason that the gas rate will rapidly decline after the CO$_2$ injection, and a quicker recharge of the driven energy is more favorable. The results for cumulative oil production show a lower recovery under CO$_2$ huff-n-puff compared to the depletion method. This behavior is resulted from the re-vaporization of the condensate dropout through the injected gas. The liquid will be “picked up” and mixed with flowing gas during huff period.

Studies have shown that a shorter huff time may be preferable for a quicker return on the investment. Therefore here we also investigate the cyclic strategy with unequal huff-n-puff period (100/50, 80/40 days for production/injection period, respectively). Moreover, we examine the scenarios where a longer depletion period (160, 120 days) is first performed, and then start for CO$_2$ huff-n-puff (80/40, 60/30 days). The corresponding results for gas and oil production are shown in Figs. 6.23 and 6.24. The cumulative CO$_2$ injection volumes are shown in Fig. 6.25. We compare the hydrocarbons recovery of different strategies in Tables 6.7 and 6.8. It is shown that the unequal huff-n-puff scheme with less injection period could lead to higher recovery enhancement, simply because the injected energy will be more
effectively utilized for a longer production time. The results also show that the strategy with a longer depletion period at the beginning could lead to better hydrocarbons recovery.

The preliminary studies indicate that there is still a large room to obtain higher enhanced recovery through optimizing the control parameters in the design of a $CO_2$ huff-n-puff injection scheme. In addition, it is expected that an improvement of oil rate can be obtained in later production period compared with the depletion method because the reduced oil viscosity combined with gradually increased oil saturation could lead to higher oil mobility and productivity. However, the relatively short simulation period adopted in this paper is just to show the potential of huff-n-puff strategy for gaining profits even in the early development stage of a gas-condensate shale reservoir.

![Graph showing gas rates of hydrocarbon components](image)

Figure 6.19: Gas rates of hydrocarbon components

| Table 6.7: Hydrocarbons recovery of the injection strategies with equal schemes |
|---------------------------------|--------|------|------|------|------|
| Hydrocarbons Production        | Base   | 140  | 100  | 80   | 60   |
| Oil ($m^3$)                    | 414.4  | 271.7| 258.4| 253.4| 248.5|
| Natural gas ($10^4m^3$)        | 24.9   | 28.6 | 29.9 | 31.2 | 31.8 |
| Injected $CO_2$ ($10^4m^3$)    | 39.2   | 48.6 | 55.3 | 57.7 |
Figure 6.20: Cumulative gas production of hydrocarbon components

Figure 6.21: Oil rates of hydrocarbon components

Table 6.8: Hydrocarbons recovery of the injection strategies with unequal schemes

<table>
<thead>
<tr>
<th>Hydrocarbons Production</th>
<th>Unequal 100/50</th>
<th>Unequal 80/40</th>
<th>First_prod_longer 160_80/40</th>
<th>First_prod_longer 120_60/30</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil ($m^3$)</td>
<td>301.9</td>
<td>282.1</td>
<td>325.9</td>
<td>303.4</td>
</tr>
<tr>
<td>Natural gas ($10^4m^3$)</td>
<td>33.7</td>
<td>33.8</td>
<td>34.5</td>
<td>35.9</td>
</tr>
<tr>
<td>Injected $CO_2$ ($10^4m^3$)</td>
<td>53.4</td>
<td>60.5</td>
<td>50.3</td>
<td>60.7</td>
</tr>
</tbody>
</table>
Figure 6.22: Cumulative oil production of hydrocarbon components

Figure 6.23: Cumulative gas production of hydrocarbon components
Figure 6.24: Cumulative oil production of hydrocarbon components

Figure 6.25: Cumulative $CO_2$ injection volumes for different cases
CHAPTER 7

SUMMARY AND CONCLUSIONS

7.1 C1-continuous Phase-Potential Upwind (C1-PPU) Schemes

It is revealed by the recent studies that in the presence of counter-current flow due to buoyancy, nonlinear convergence problems may be pronounced when the popular PPU scheme is used to approximate the numerical flux. The PPU numerical flux is non-differentiable across the co-current/counter-current flow regimes and thus may lead to oscillations or even divergence in the Newton iterations. In the design of numerical flux calculations for transport problems, both the level of nonlinearity and the C1-continuity can have dramatic effects on the nonlinear convergence of the solution for the timestep. Recently proposed methods address improved smoothness of the numerical flux.

We devise and analyze an alternative numerical flux scheme called C1-PPU that allows a smooth variation between the co-current/counter-current flow regimes as well as an optimal balance between the scalar nonlinearity and accuracy of the flux function. C1-PPU involves a novel use of the flux limiter concept from the context of high-resolution methods. The scheme is general and applies to the fully coupled formulation of mass conservation equations for an arbitrary number of phases.

We derive saturation and pressure estimates for a proof of the solution existence to the proposed scheme. Several numerical examples for two- and three-phase flows in heterogeneous and multi-dimensional reservoirs are presented. The results show that the C1-PPU scheme exhibits superior convergence properties for large time steps. In some cases with fully-coupled flow and transport, C1-PPU achieves reduction in the total Newton iterations by more than an order of magnitude compared with PPU.
The generalized C1-PPU scheme is continuously differentiable with respect to saturations as well as phase potentials. This property is expected to further help in the scenarios where total velocities vary significantly in time or abrupt changes of boundary conditions (e.g., changes in wells) are present.

### 7.2 Multislope MUSCL Method

We present a fully-implicit CCFV framework that can achieve second-order spatial accuracy on smooth solutions, while at the same time maintain robustness and nonlinear convergence performance. We develop a novel multislope MUSCL method and an adaptive limiting strategy that have improved computational efficiency, smoothness and accuracy. In contrast to the classical monoslope method in which a unique limited gradient is used for a given element, the multislope method performs the limiting in 1-D situations for each edge. The novel multislope scheme interpolates the required values at the edge centroids in a simple way by taking advantage of some geometric features of the triangular mesh. The numerical diffusion caused by mesh skewness is largely reduced and optimal second order accuracy can be achieved without sacrificing robustness. An improved smooth piecewise-linear limiter is developed to prevent spurious oscillations on non-uniform mesh.

Grid convergence studies and several numerical tests with discrete fractured system are carried out to demonstrate the accuracy and robustness of the numerical model. The results show that the high-order MUSCL method effectively reduces numerical diffusion, leading to improved resolution of saturation fronts compared with the first-order method. The developed multislope method exhibits superior nonlinear convergence compared with another alternative.

### 7.3 Improved Projection-based EDFM Model

In this topic we show that the EDFM approach has significant limitations for representing the multiphase displacements across a fracture, due to its incapability to capture the proper flux split through a fracture. The limitations could induce large errors on the
displacement efficiency predictions of improved oil recovery processes for NFRs. Here we provide a detailed analysis for the flow process of EDFM to illuminate when and why the method fails. The analysis motivates us to exploit pEDFM as a promising method to resolve the limitations associated with EDFM. pEDFM is recently proposed by Tene et al. (2016) and is based on the introduction of additional $f - m$ flux connections. The method is originally designed for accurately modeling the effect of the lower-dimensional features with a wide range of permeabilities (e.g. flow barriers).

We present one extension and two improvements for the pEDFM approach. Through several simulation examples we illustrate that with a naive implementation of pEDFM, undesirable degradations in numerical solutions may occur. It is observed that unphysical configurations of the extended fracture-matrix connections can be created in the naive implementation. A simple but effective way is proposed to resolve this issue by imposing a constraint on the preprocessing stage for creating the extended connections.

We establish a number of test cases with different fracture distributions to benchmark the performances of the new EDFM method for multiphase flow. The comparison results demonstrate that the improved pEDFM method significantly outperforms the original EDFM method. Grid convergence studies are also performed for different numerical schemes. Compared to the first-order convergence rate of the improved pEDFM and unstructured DFM methods, EDFM shows an almost zeroth-order convergence. In addition, improved pEDFM has a similar performance with the unstructured DFM method, which is very desirable for an embedded type of method.

Although the current numerical examples are based on the simplified model for immiscible two-phase flow, the improved pEDFM method can be readily applied to more realistic and complex systems with multiphase multicomponent (compositional) fluids. Also, the new method developed can be extended to 3D implementations without any difficulty. Our future works include 3D simulations of compositional fluid flows with buoyancy and capillarity.
7.4 Coupled Flow and Geomechanics Modeling

During gas depletion, the net change of shale porosity and permeability is the outcome of the several competing processes, including the non-Darcy flow, pore space reduction due to the adsorbed layer, gas desorption and changes in effective stress. The flow and stress-sensitive behaviors are further exacerbated by the creation of complex fracture network during hydraulic fracturing. Proppants are injected with fracturing fluid to maintain the fracture conductivity. Under the effects of pressure decline and high confining stresses on the fracture faces, proppant compaction, embedment and even crushing may occur, causing fracture closure and thus significant production loss.

We present a fully coupled fluid flow and geomechanics model to simulate the complex production phenomena in fractured shale gas reservoirs. The MFD method is applied for the discretization of fluid flow and the finite-element for mechanics. The conformal unstructured grid is used to explicitly represent the discrete fractures, whose mechanics behavior is handled through a splitting-node technique. We also develop a comprehensive proppant-fracture model which is based on the elasto-plastic contact mechanics, to accurately characterize the complex interactions between proppant and fracture.

Sensitivity studies are conducted to investigate which factors have significant impacts on well performance and gas recovery of shale formations. High fidelity numerical solutions are provided to simulate the rate-transient variations in the presence of the different flow and geomechanical mechanisms.

7.5 Compositional Modeling

This work develops comprehensive simulation capabilities to understand and predict complex transport processes and phase behavior associated with the production behavior in gas-condensate shale reservoirs. Related storage and transport mechanisms such as multi-component apparent permeability (MAP), sorption and molecular diffusion are considered. In order to accurately capture the complicated phase behavior of the multiphase fluids, an EOS-based phase package is incorporated into the simulator. Capillary pressure is coupled
with phase equilibrium equations, and the resulting system of nonlinear fugacity equations
is solved to examine the effect of nanosize pores on dew-point pressures. We could obtain
following conclusions from the simulation results in this study:

1) Lighter components have larger flow capacity and the valuable heavy components will
be left behind in the formation during production. The results illustrate that the multiple
components effect should be captured by the MAP model instead of using a single pseudo-
component apparent permeability;

2) Desorption has large impact on well performance and could be an important storage
mechanism for heavy hydrocarbon fractions, which contributes significantly to condensate
production;

3) Large capillary pressure has significant effects on phase behaviors, which cannot be ignored
for reliable modeling of gas-condensate shale reservoirs. The elevated dew point pressure in
the fluid system leads to more condensate dropout and thus higher oil saturation. In con-
trast, gas rate is lower under the effect of capillary pressure due to the reduction in gas
relative permeability caused by more significant condensate blockage;

4) The unequal huff-n-puff scheme with less injection period could lead to higher recovery
enhancement, because the injected energy will be more effectively utilized for a longer pro-
duction time. The results also show that the strategy with a longer depletion period at the
beginning could lead to better hydrocarbons recovery;

5) The preliminary simulation studies show that CO2 huff-n-puff injection strategy has the
potential for gaining profits even in the early development stage of a gas-condensate shale
reservoir. It is also shown that there is still a large room to obtain higher enhanced recovery
through optimizing the control parameters in the design of a huff-n-puff scheme.
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