FLUID INJECTION AND MIGRATION IN THE SUBSURFACE: REDUCED-ORDER MODELS AND MULTISCALE MODELING APPROACHES

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Abstract

Carbon capture and storage (CCS) has been identified as the only climate mitigation option that can significantly reduce anthropogenic CO$_2$ emissions while allowing continued use of fossil fuels for electricity generation and other industrial processes. CCS involves permanent sequestration of the CO$_2$ captured from burning of fossil fuels into deep geologic formations. This dissertation studies the two-phase flow dynamics of geologic CO$_2$ sequestration, as well as other subsurface fluid injections, including acid gas injection, liquid waste disposal and enhanced oil recovery; and develops a series of computational multi-phase flow models with a broad range of complexity to understand and predict injection and migration of the various kinds of fluid injections in the subsurface.

Chapter 2 studies the axisymmetric flows generated from injection of one fluid into a horizontal confined porous medium originally filled with another fluid using the reduced-order vertical equilibrium and sharp interface assumptions, where four asymptotic analytical solutions and an associated flow regime diagram distinguishing the different solutions are obtained. Chapter 3 identifies the kinds of solutions appropriate for practical CO$_2$ injection projects as well as other subsurface fluid injection applications. The analytical solutions and the flow regime diagram provide a simple guidance tool for expected behaviors of the different injection operations.

Chapters 4 and 5 report novel multiscale numerical algorithms and a range of vertically-integrated models that can model the two-phase flow dynamics of CO$_2$ and brine in both homogeneous and layered heterogeneous geologic formations. The capability to capture the additional two-phase flow dynamics in the vertical dimension, while maintaining much of the computational advantages of the conventional vertical equilibrium models makes these multiscale models very attractive for computational studies of large-scale CO$_2$ storage systems.

Chapter 6 highlights some interesting extensions to more advanced models from the multiscale algorithm developed in Chapters 4 and 5. One extension is a set of hybrid
vertically-integrated multi-layer and multi-dimensional models for CO\textsubscript{2} sequestration in geologic formations with complex geologic structures and other energy and environment systems involving subsurface fluid injection. The other extension is a set of vertically-integrated dual-porosity dual-permeability models for modeling of geologic CO\textsubscript{2} sequestration in fractured reservoirs.
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5.4 \( \text{CO}_2 \) plume comparison between the MLDR model and TOUGH2 for a two-layer formation with permeability of 1 mD and 100 mD in the upper and lower layers, respectively. The first row shows the \( \text{CO}_2 \) plume from the MLDR model and the second row shows that from TOUGH2. The plumes in the left column are after 1 year of injection and those in the right column are after 5 years of injection.
5.5 **CO$_2$ plume comparison between the MLDR model and TOUGH2 for a**

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5.6 **CO$_2$ plume comparison between the MLDR model and TOUGH2 for a**

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Chapter 1

Introduction

1.1 Global warming

Scientific evidence shows that climate is changing and that these changes are largely caused by human activities ([IPCC] 2014). The anthropogenic activity of most concern is the continuing emission of carbon dioxide (CO₂) into the atmosphere. From 1958 to February 2016, the CO₂ concentration in the atmosphere measured at Mauna Loa Observatory, Hawaii (Figure 1.1) has increased from 315 parts per million by volume (ppmv) to 403 ppmv ([Scripps Institution of Oceanography] 2016). The annual global CO₂ emissions from fossil fuels combustion and other industry processes have reached 35.9 ± 1.8 Gt in 2014 ([Quéré et al.] 2015), with the power sector being the major contributor. According to the IPCC Fifth Assessment Report ([IPCC] 2014), tremendous amounts of CO₂ emissions reduction have to occur to limit the global mean temperature to 2 degrees Celsius (°C) above the pre-industrial levels by the end of this century (see Figure 1.2). Cumulatively, no more than about 1,200 Gt CO₂ should be emitted to the atmosphere between 2015 and the end of the century to meet the 2 °C target ([Fuss et al.] 2014). While a number of technologies exist that can help meet this target (see Section 1.2), the extent to which those technologies
Figure 1.1: CO₂ concentration in the atmosphere measured at Mauna Loa Observatory, Hawaii (from Scripps CO₂ Program).

will be implemented depends on many other factors including both economic and political considerations.

1.2 Carbon capture and storage

A portfolio of technologies exists to meet the world’s energy needs while limiting CO₂ emissions to meet the 2 degree C target ([Pacala and Socolow](2004), [IPCC](2005, 2014)). One such technology is Carbon Capture and Storage (CCS), a technology that allows use of fossil fuels for electrical power generation and other industrial processes while reducing CO₂ emissions by capturing the CO₂ produced by combustion and then storing the captured CO₂ in the deep subsurface of the Earth. According to [International Energy Agency](2015), CCS can deliver 13% of the accumulative CO₂ emission reduction by 2050 to limit the
temperature increase to 2 °C. CCS involves two major parts: capture and storage. Capture of CO₂ can occur at large-scale stationary sources, such as fossil fuel (coal or gas) fired power plants, biomass power plants, and industrial cement factories. For CO₂ storage, the most likely locations are deep geological formations, in particular sedimentary basins. Within sedimentary basins, possible storage formations include depleted oil fields, depleted gas fields, deep coal seams and saline aquifers (IPCC, 2005). These geological storage options have large storage capacities. IPCC (2005) shows that the total capacity appears to be more than adequate, with the capacity of saline aquifers being the largest at about 1000 Gt. Another study by Szulczewski et al. (2012) suggests that CCS in the United States can store enough CO₂ to stabilize emissions at the level of the year 2012 for at least 100 years.

To date, CCS has not been implemented at scales necessary to tackle global warming. This is due to various factors, including the high cost of capture and the lack of government policies that place a cost on atmospheric emissions. However, because most climate mitigation scenarios include the large-scale deployment of CCS (IPCC, 2014; International...
Energy Agency [2015], it remains important to study the implementation logistics and potential environmental consequences of large-scale implementation.

1.3 Geologic CO2 sequestration in saline aquifers

Deep saline aquifers are considered as the most likely target for large-scale geologic carbon sequestration due to their large storage capacity and availability throughout the world (IPCC, 2005; Celia et al., 2015). This section identifies the key physical and chemical mechanisms of the CO2 injection system in saline aquifers, the practical questions that need to be answered, and the challenges of the computational modeling studies.

In geologic CO2 sequestration in saline aquifers, CO2 is injected into the saline aquifer through either vertical or horizontal wells. Injection depths are usually chosen so that the injected CO2 is in its supercritical state. While the supercritical CO2 has density much larger than gaseous CO2, that density is still small compared to the density of the resident brine, with the difference ranging from 250 kg/m3 to up to 950 kg/m3, depending on formation depth, geothermal gradients, pressure gradient, surface temperature and brine salinity (Nordbotten and Celia, 2012). The injected CO2 is always less viscous than brine, and the associated viscosity contrasts between the two fluids range from 0.026 to 0.2. The resident brine is often considered to be the wetting fluid, and the injected CO2 is the nonwetting fluid. A range of physical and chemical mechanisms are involved in the CO2 injection system. When CO2 is injected into the saline aquifer, it will migrate horizontally driven by the pressure gradient from injection, as well as migrating upward driven by buoyancy due to the density difference between the injected CO2 and the resident brine. CO2 continues to move upward until it reaches a barrier, typically a low-permeability caprock. Injecting CO2 into a saline aquifer can also lead to chemical reactions, e.g. CO2 dissolution into brine and H2O evaporation into the CO2 phase, and aqueous geochemical reactions that may eventually result in the precipitation and dissolution of the host rock minerals. Pushing CO2 into
the aquifer also increases the pore pressure of the aquifer and thereby changes the stress conditions of the geologic formation, which may cause a sequence of mechanical reactions, such as reactivation of existing faults or creation of new faults in the caprock, and inducing seismic events. Sometimes, the injected CO$_2$ may have a significantly different temperature than the aquifer, leading to thermal effects, such as, changes in the fluid properties, and changes in the stress regimes of the aquifer and caprock. The extent to which any of these possible consequences of injection is important depends on the injection conditions and rock properties.

### 1.3.1 Practical questions

To safely storage large amounts of CO$_2$ in a saline aquifer for long time periods, e.g. on the order of thousands of years, a range of practical questions need to be answered, including

(IPCC, 2005; De Coninck and Benson, 2014; Celia et al., 2015)

1. What is the storage capacity of a saline aquifer?

2. What are the pressure buildup and injectivity?

3. What are the leakage risk and the associated mitigation strategy?
1.3.2 Modeling challenges

Computational models are routinely used to answer the identified practical questions, especially for questions related to fluid migration and pressure increase. Modeling the subsurface system of CO\textsubscript{2} injection can be challenging as it involves a variety of different physical and chemical processes at different spatial and temporal scales. In addition, the physical systems often have large spatial extent and therefore require a large number of grid cells for numerical models, especially when the small-scale heterogeneities are important and need to be represented, leading to significant computational demand. The usual data scarcity of the subsurface makes it even more challenging, because computational models need to be run multiple times (sometimes hundreds to thousands of times) with different geological inputs to understand the uncertainties in the modeling results.

Computational models with different levels of complexities have been developed in the past decade. Bandilla et al. (2015) categorizes these models as: coupled three-dimensional models, simplified multiphase three-dimensional models, vertical equilibrium models, and simplified vertical equilibrium models. Coupled three-dimensional models involve multiphase flow, geochemistry and geomechanics and solve them in three dimensions. The simplified multiphase three-dimensional models focus on the process of multiphase flow and transport, usually neglecting geochemistry and geomechanics. The vertical equilibrium models are reduced-dimension models based on vertical integration and the vertical pressure equilibrium assumption. Vertical equilibrium models can be further simplified by assuming a macroscopic sharp interface between CO\textsubscript{2} and brine, and assuming simple geometries, i.e. horizontal homogeneous geologic formation. These simplified vertical equilibrium models usually have analytical or semi-analytical solutions. Detailed discussion of these models can be found in Bandilla et al. (2015).

One advantage of the vertical equilibrium models and the subsequent semi-analytical and analytical models is that they are computationally very efficient owing to the dimension reduction from vertical integration. Early literature of vertical equilibrium models exists in...
the hydrology community, e.g. [Bear (1972)], the petroleum community, e.g. [Lake (1989)], and the fluid mechanics community, e.g. [Huppert and Woods (1995)]. In the last decade, vertical equilibrium models have been developed for modeling geologic CO\textsubscript{2} sequestration. These include simplified vertical equilibrium models that can be solved analytically (see, e.g. [Pritchard et al., 2001; Lyle et al., 2005; Nordbotten and Celia, 2006; Verdon and Woods, 2007; Hesse et al., 2008; MacMinn et al., 2010; Juanes et al., 2010]); semi-analytical models that can model injection wells and leakage pathways (see, e.g. [Nordbotten et al., 2009; Kang et al., 2014]); and numerical models that can include various complex features, e.g. capillary pressure, geologic tomography, solubility trapping, fluid compressibility, etc. (see, e.g. [Gasda et al., 2009; 2011; 2012a; Andersen et al., 2015]). The applicability of the vertical equilibrium assumptions have been discussed in [Lake (1989), Yortsos (1995), Nordbotten and Dahle (2011)], and from a more practical viewpoint in [Court et al., 2012]. These vertical equilibrium models have been applied to both site-scale and basin-scale problems to answer practical questions (see, e.g. [Celia et al., 2011; Nilsen et al., 2011; Gasda et al., 2012b; Bandilla et al., 2012; Grude et al., 2014; Huang et al., 2014]).

Despite the development of models with various levels of complexity, there are still substantial gaps in the literature. The work in this thesis provides new information and insights for two such gaps. First, although various analytical solutions have been developed for the simplified vertical equilibrium models, it is not clear when to use which solutions, especially in terms of the interplay between different driving forces (the force from injection and buoyancy) for CO\textsubscript{2} injection into a confined aquifer. Second, the vertical equilibrium assumption significantly simplifies the problem, but it is a very strict assumption which is invalid for a number of practical situations. For instance, the vertical equilibrium assumption may not be valid for geologic formations with relatively low vertical permeability and/or heterogeneous permeability distribution, because for these cases the time required for vertical equilibrium to be reached may be large relative to the simulation time, thereby invalidating the assumption ([Court et al., 2012]). For these kinds of problems, more
advanced vertically-integrated models are needed if a simplified approach (vertical integration) is to be used. These two research gaps largely motivate this dissertation. Section 1.5 will elaborate the specific research questions we try to answer and the specific research objectives.

## 1.4 Other fluid injections into the deep subsurface

Fluid injection into the deep subsurface has been used for many other engineering practices, which have modeling challenges similar to geologic CO$_2$ sequestration. Here, we highlight three of them: CO$_2$ - enhanced oil recovery (EOR), deep well liquid waste disposal and acid gas injection.

CO$_2$ - EOR is a technique to increase the amount of crude oil that can be produced from an oil field. This technique enhances oil production by injecting CO$_2$ into a reservoir to push additional oil to a production well, the process of which is often called CO$_2$ flooding. Usually, CO$_2$ flooding involves injection of volumes of CO$_2$ alternating with injection of volumes of water, which is referred to as water alternating (WAG) - EOR. The WAG-EOR technique helps to mitigate the viscous fingering of the injected CO$_2$, which can reduce the sweep efficiency of the process (Lake, 1989).

The practice of deep well liquid waste disposal injects various types of wastes into the deep subsurface, including hazardous industrial wastes, non-hazardous industrial wastes, and municipal wastewater. The wells are typically drilled hundreds of meters below the lowermost underground source of drinking water. Currently, there are approximately 800 operational wells in the United States (U.S. EPA, 2016). These wells are classified as class I wells by EPA, as part of the EPA regulations that protect underground sources of drinking water under the Underground Injection Control (UIC) program.

Acid gas injection is a practice in the oil and gas industry, especially in Canada, used to dispose the acid gas (a mixture of H$_2$S and CO$_2$) that is separated from oil and gas produced
from “sour” hydrocarbon reservoirs in the deep geologic formations (Bachu et al., 2003). In 2009, 48 wells were used for the disposal of produced acid gas in Canada.

In any analysis of these kinds of injection systems, prediction of where both the injected and the displaced (resident) fluids migrate over time is needed. This dissertation develops tools to address questions related to fluid migration for these three types of fluid injection operations, using the computational tools we develop for CO₂ sequestration.

1.5 Contributions of this dissertation

This section highlights the contributions of this dissertation and provides an overview of the chapters. The dissertation addresses the two main research gaps identified in Section 1.3. The first part of the dissertation (Chapters 2 & 3) considers the reduced-order simplified vertical equilibrium models, obtaining a complete set of asymptotic analytical solutions and developing a flow regime diagram that distinguishes the various analytical solutions in the asymptotic limits. Data from the literature are collected and analyzed to identify the kinds of solutions appropriate for practical CO₂ injection projects as well as other subsurface fluid injection applications. The second part of the dissertation (Chapters 4 & 5) goes beyond the vertical equilibrium models and develops a family of advanced vertically-integrated models that do not rely on the vertical equilibrium assumption. These models provide a set of computational tools that give accurate results for cases with significant vertical flow dynamics, while still being much more computationally efficient compared to full three-dimensional models. Chapter 6 presents an extensive discussion of the future extensions of the models.

Chapter 2 presents a theoretical analysis of the reduced-order sharp-interface vertical equilibrium model for an axisymmetric system with an injected fluid displacing a resident fluid, not necessarily CO₂ and brine. It reports a complete set of analytical solutions for
this axisymmetric flow problem and a flow regime diagram that characterizes the fluid flow system and specifies conditions under which each of the analytical solutions applies.

Chapter 3 uses the derived theoretical results from Chapter 2 to identify the kinds of solutions appropriate for a range of practical subsurface fluid injection applications, including geologic CO$_2$ sequestration, WAG-EOR, deep well liquid waste disposal, and acid gas injection. The analysis provides a simple guidance tool for expected behavior of the different injection operations.

Chapter 4 reports a novel vertically-integrated model that is capable of capturing the vertical two-phase flow dynamics of CO$_2$ and brine in a homogeneous geologic formation. The model is developed in a multi-scale framework and is referred to, using the terminology from multi-scale modeling, as “single-layer dynamic reconstruction” model.

Chapter 5 extends the numerical algorithm developed in Chapter 4 to allow simulation of CO$_2$ and brine migration in layered heterogeneous geologic formations. This new algorithm is referred to as a “multi-layer dynamic reconstruction” model. This multi-layer dynamic reconstruction model is an attractive computational tool for simulations of large-scale CO$_2$ injection and migration in layered geologic formations because of its computational efficiency.

Chapter 6 discusses model extensions based on the multiscale numerical algorithms developed in Chapters 4 and 5. The first extension involves two hybrid models constructed by combining the vertical equilibrium model, dynamic reconstruction algorithms and other models. The first hybrid model is a multi-layer vertically-integrated framework that uses different models for different layers and couples the layers in the vertical direction, while the second hybrid model is a multi-dimensional model that couples the vertical equilibrium model, the dynamic reconstruction and the full three-dimensional model in the horizontal direction. These two hybrid models provide efficient computational tools that are attractive for CO$_2$ and brine migration in geologic formations with complex structures. The second extension is a range of vertically-integrated dual-porosity dual-permeability models for
CO₂ injection into fractured reservoirs, the numerical algorithms of which follow closely with the dynamic reconstruction framework.

Chapter 7 summarizes the dissertation and discusses the significance of the findings.

1.6 Publications

The core chapters of this dissertation (Chapters 2 through 6) have either been published or (will be) submitted for publication. Below are the full references:


Chapter 2

Axisymmetric Flows from Fluid Injection into a Confined Porous Medium

This chapter was adopted from the publication [Guo et al. (2016)]:


[Guo et al. (2016)] is a follow-up study of another co-authored publication [Zheng et al. (2015a)]:


2.1 Abstract

We study the axisymmetric flows generated from fluid injection into a horizontal confined porous medium that is originally saturated with another fluid of different density and viscosity. Neglecting the effects of surface tension and fluid mixing, we use the lubrication
approximation to obtain a nonlinear advection-diffusion equation that describes the time evolution of the sharp fluid-fluid interface. The flow behaviors are controlled by two dimensionless groups: $M$, the viscosity ratio of displaced fluid relative to injected fluid, and $\Gamma$, which measures the relative importance of buoyancy and fluid injection. For this axisymmetric geometry, the similarity solution involving $R^2/T$ (where $R$ is the dimensionless radial coordinate and $T$ is the dimensionless time) is an exact solution to the nonlinear governing equation for all time. Four analytical expressions are identified as asymptotic approximations (two of which are new solutions): (i) injection-driven flow with the injected fluid being more viscous than the displaced fluid ($\Gamma \ll 1$ and $M < 1$) where we identify a self-similar solution that indicates a parabolic interface shape; (ii) injection-driven flow with injected and displaced fluids of equal viscosity ($\Gamma \ll 1$ and $M = 1$), where we find a self-similar solution that predicts a distinct parabolic interface shape; (iii) injection-driven flow with a less viscous injected fluid ($\Gamma \ll 1$ and $M > 1$) for which there is a rarefaction wave solution, assuming that the Saffman-Taylor instability does not occur at the reservoir scale; and (iv) buoyancy-driven flow ($\Gamma \gg 1$) for which there is a well-known self-similar solution corresponding to gravity currents in an unconfined porous medium (Lyle et al., 2005). The various axisymmetric flows are summarized in a $\Gamma-M$ regime diagram with five distinct dynamic behaviors including the four asymptotic regimes and an intermediate regime. The implications of the regime diagram are discussed using practical engineering projects of geological CO$_2$ sequestration, enhanced oil recovery, and underground waste disposal.

2.2 Introduction

The propagation of viscous gravity currents occurs in a variety of geophysical and industrial contexts, for example, the propagation of magma, geological CO$_2$ sequestration, underground thermal energy storage, enhanced oil recovery, and underground waste disposal.
There have been numerous studies on the flow of viscous gravity currents with geometries and driving forces inspired by these applications. It is common to simplify the system by assuming that the injected and displaced fluids are segregated due to strong buoyancy effects and reach equilibrium in the vertical direction. Here, we invoke this vertical equilibrium assumption and focus on the axisymmetric propagation that is of practical interest, especially in reservoir engineering where various fluids are frequently injected underground through vertical wells; approximately axisymmetric flows are expected to be generated following fluid injection. A summary of previous studies on axisymmetric flows driven by buoyancy and/or fluid injection is provided in Table 2.1, including characterization of spreading rates in terms of similarity solutions of the first kind, where spreading occurs outward, and the second kind, where spreading occurs inward.

When a viscous dense gravity current spreads axisymmetrically above a horizontal impermeable substrate, it is common to analyze the flow using the lubrication approximation, which leads to a nonlinear diffusion equation that describes the time evolution of the free interface (see, e.g., Huppert, 1982; Didden and Maxworthy, 1982). Self-similar solutions have been obtained to describe the fluid flow subject to both constant total volume and constant injection rate, and laboratory experiments have been conducted to verify the applicability of the self-similar solutions. Axisymmetric viscous gravity currents spreading over an elastic membrane has also been studied; a transition from an early-time similarity to a late-time similarity was identified to characterize the spreading dynamics (Zheng et al., 2015b). An analogous situation is the axisymmetric spreading of a gravity current in an unconfined porous medium, and self-similar solutions have been obtained and verified using experiments in a porous medium of packed beads (Lyle et al., 2005). A two-phase model has also been proposed to describe the axisymmetric spreading of a viscous gravity current (Golding et al., 2013), including the effect of interfacial tension. In addition, a second-kind self-similar solution has been obtained for the inward spreading of an axisymmetric grav-
<table>
<thead>
<tr>
<th>Flow conditions</th>
<th>Front propagation laws</th>
<th>Experiments</th>
<th>References</th>
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</thead>
<tbody>
<tr>
<td>in atmosphere, unconfined, outward flow</td>
<td>$r \propto t^{1/8}$ (constant volume), $r \propto t^{1/2}$ (constant injection)</td>
<td>Yes, Yes</td>
<td>Huppert (1982), Didden and Maxworthy (1982)</td>
</tr>
<tr>
<td>in atmosphere, unconfined, outward flow</td>
<td>$r \propto t^{1/2}$ (at early times), $r \propto t^{1/4}$ (at late times) (over elastic substrate)</td>
<td>Yes</td>
<td>Zheng et al. (2015b)</td>
</tr>
<tr>
<td>in atmosphere, unconfined, inward flow</td>
<td>$r \propto (t_c - t)^{0.762...*}$ (second kind self-similarity)</td>
<td>Yes</td>
<td>Gratton and Minotti (1990), Diez et al. (1992)</td>
</tr>
<tr>
<td>in atmosphere, unconfined, inward flow</td>
<td>$r \propto (t_c - t)^{0.762...**}$ (second kind self-similarity) (with slow vertical drainage)</td>
<td>Yes</td>
<td>Zheng et al. (2015c)</td>
</tr>
<tr>
<td>porous media, unconfined, outward flow</td>
<td>$r \propto t^{1/4}$ (constant volume), $r \propto t^{1/2}$ (constant injection)</td>
<td>No, Yes</td>
<td>Lyle et al. (2005), Zheng et al. (2014)</td>
</tr>
<tr>
<td>porous media, unconfined, inward flow</td>
<td>(second kind self-similarity)</td>
<td>No</td>
<td>Golding et al. (2013)</td>
</tr>
<tr>
<td>porous media, unconfined, outward flow</td>
<td>$r \propto t^{1/2}$ (constant injection) (two-phase gravity currents)</td>
<td>No</td>
<td>Pritchard et al. (2001), Spannuth et al. (2009)</td>
</tr>
<tr>
<td>porous media, unconfined, outward flow</td>
<td>$r \rightarrow$ finite maximum length (with slow vertical drainage)</td>
<td>Yes</td>
<td>Pritchard et al. (2001), Spannuth et al. (2009)</td>
</tr>
<tr>
<td>porous media, confined, outward flow</td>
<td>$r \propto t^{1/2}$ (constant injection) (rarefaction wave solution)</td>
<td>No</td>
<td>Nordbotten and Celia (2006)</td>
</tr>
<tr>
<td>porous media, confined, outward flow</td>
<td>$r \propto t^{1/2}$ (constant injection) (five distinct flow regimes)</td>
<td>No</td>
<td>current work</td>
</tr>
</tbody>
</table>

Table 2.1: Summary of axisymmetric viscous gravity currents in unconfined and confined geometries. The front propagation laws are also included in this table with $r$ representing the length of the current and $t$ representing time. *For an inward spreading viscous gravity current, a second-kind self-similar solution is obtained with $t_c$ denoting the time for the front to reach the origin; the scaling exponent is an irrational number obtained by solving a nonlinear eigenvalue problem. **With vertical fluid drainage, a mathematical transform from $t$ to $\tau$ is introduced (see, e.g., Murray (1989), Pritchard et al. (2001), Zheng et al. (2015c)).
ity current \cite{Gratton1990, Diez1992}, where the scaling exponents are determined by solving a nonlinear eigenvalue problem \cite[e.g.,][]{Barenblatt1979, Sedov1993}.

When the substrate is permeable, vertical drainage occurs during the horizontal spreading of an axisymmetric gravity current. In this situation, the horizontal spreading of a gravity current approaches a steady state under constant fluid injection and the fluid-fluid interface reaches a finite maximum horizontal extent; without fluid injection (constant total volume), the length of a gravity current first reaches a maximum value and eventually decreases because of fluid loss through the permeable substrate \cite[e.g.,][]{Pritchard2001, Spannuth2009}. For inward spreading of gravity currents on thin permeable substrates, a second-kind self-similar solution can be obtained by introducing a mathematical transform to map the problem to the analogous flow situation without fluid drainage \cite{Zheng2015c}. If the horizontal substrate is subjected to sites of local drainage, for example a fault, the gravity current no longer spreads in an axisymmetric pattern because of the localized fluid loss \cite[e.g.,][]{Neufeld2011, Vella2011}. Breaking of symmetry can also occur if a gravity current spreads above a substrate that is tilted from the horizontal direction \cite{Lister1992, Vella2006}.

For confined geometries, there are fewer studies on the propagation of axisymmetric gravity currents from fluid injection, although there have been many studies in confined Cartesian geometries \cite[e.g.,][]{Bear1972, Huppert1995, Hesse2007, Hesse2008, Verdon2007, Hallez2009, Taghavi2009, MacMinn2010, MacMinn2011, Matson2012, Saha2013, MacMinn2014, Pegler2014, Zheng2015a, Zheng2015d}. For an axisymmetric flow, considering the movement of the displaced fluid that initially saturates the porous medium, a nonlinear advection-diffusion equation describes the dynamics of the fluid-fluid interface under constant fluid injection, and a rarefaction wave solution has been obtained when the injected fluid is less viscous than the displaced fluid \cite{Nordbotten2006, Nordbotten2012}.  


In this chapter, we extend the previous work of Nordbotten and Celia (2006) on the axisymmetric flow from constant fluid injection into a confined porous medium, and provide new approximate analytical solutions when the injected fluid is equally viscous or more viscous, compared with the displaced fluid.

In structuring this chapter, we begin in Section 2.3 with the derivation, in cylindrical coordinates, of the nonlinear advection-diffusion equation that describes the time evolution of the axisymmetric fluid-fluid interface. In Section 2.4, we study the injection-dominated regimes and show three different analytical expressions for the spreading dynamics, which depend on the viscosity ratio of the injected and displaced fluids. In Section 2.5, we study the buoyancy-dominated regime, which recovers the flow behaviors in an unconfined porous medium. We summarize in Section 2.6 our major findings in a regime diagram of five distinct flow behaviors that links the well-known analytical results from previous studies (Lyle et al., 2005; Nordbotten and Celia, 2006) and new analytical solutions from the current study. We investigate in Section 2.7 the transition process to develop the various self-similar solutions, and we discuss the implications for practical engineering applications in Section 2.8. The chapter concludes in Section 2.9 with a summary of major findings and more discussion of the model assumptions.
2.3 Theoretical model

We study the axisymmetric flow as fluid injection occurs in a horizontal confined porous medium of thickness $h_0$, where both the upper and lower boundaries are impermeable, see Figure 2.1. The porous medium is assumed to be isotropic and homogeneous with constant permeability $k$ and porosity $\phi$. Also, the flow is assumed to be axisymmetric; hence we use cylindrical coordinates $(r, z)$ with $r = 0$ corresponding to the location of the injection well, and we assume the radius of the well is negligibly small. We assume that the two fluids are immiscible and we neglect the effect of interfacial tension. Then, the two fluid phases are separated by a sharp interface and we denote the thickness of the injected fluid by $h(r,t)$. The injected fluid has density $\rho_i$ and viscosity $\mu_i$; the displaced fluid has density $\rho_d$ and viscosity $\mu_d$. Without loss of generality, we assume the injected fluid is less dense than the displaced fluid, and we define the fluid density difference as $\Delta \rho = \rho_d - \rho_i > 0$. A schematic of the flow system is shown in Figure 2.1.

When the aspect ratio (height relative to length) of the fluid-fluid interface is small, the flow is mainly horizontal, and it is natural to analyze the flow using the lubrication approximation. Then, the vertical velocity is negligible, and the fluid pressure exhibits a hydrostatic distribution:

\begin{align}
 p_i(r, z, t) &= p_0(r, t) + \rho_i gz, \quad \text{for} \quad 0 \leq z \leq h(r, t), \quad (2.1a) \\
 p_d(r, z, t) &= p_0(r, t) + \rho_i gh(r, t) + \rho_d g(z - h(r, t)), \quad \text{for} \quad h(r, t) < z \leq h_0, \quad (2.1b)
\end{align}

where $p_0(r, t)$ is the pressure at the top of the porous medium, and $z$ is positive downward.

The horizontal (radial) velocities in the two fluids can be calculated using Darcy’s law

\begin{align}
 u_i &= -\frac{k}{\mu_i} \frac{\partial p_i}{\partial r} \quad \text{and} \quad u_d = -\frac{k}{\mu_d} \frac{\partial p_d}{\partial r}, \quad (2.2a, b)
\end{align}
Also, the local continuity equations are given by

\[ \phi \frac{\partial h}{\partial t} + \frac{1}{r} \frac{\partial (rhu_i)}{\partial r} = 0, \quad (2.3a) \]

\[ \phi \frac{\partial (h_0 - h)}{\partial t} + \frac{1}{r} \frac{\partial (r(h_0 - h)u_d)}{\partial r} = 0, \quad (2.3b) \]

which can be summed and integrated radially to obtain

\[ hu_i + (h_0 - h)u_d = \frac{q}{2\pi r}, \quad (2.4) \]

where \( q \) is the volumetric injection rate through the injection well. In this chapter, we only consider the case of constant fluid injection, i.e., \( q \) is a constant.

In addition, the global mass constraint then requires:

\[ 2\pi \phi \int_0^{r_{N_1}(t)} rh(r,t)dr = qt, \quad (2.5) \]

where \( r_{N_1}(t) \) denotes the furthest radial extent of the front (see Figure 2.1). Using Equation (2.3), it can be shown that Equation (2.5) is equivalent to Equation (2.4).

Combining Equations (2.1) to (2.4), we obtain a nonlinear advection-diffusion equation that governs the space-time evolution of the fluid-fluid interface \( h(r,t) \):

\[ \frac{\partial h}{\partial t} = \frac{1}{\phi r} \frac{\partial}{\partial r} \left( \frac{\Delta \rho gh(h_0 - h)r}{\mu_d h + \mu_i (h_0 - h)} \frac{\partial h}{\partial r} + \frac{q \mu_i (h_0 - h)}{2\pi (\mu_d h + \mu_i (h_0 - h))} \right). \quad (2.6) \]

We note that a similar equation has been derived by Nordbotten and Celia (2006), who also considered the effect of constant residual saturation. The analogous equation for the case of constant fluid injection in Cartesian geometries was presented and analyzed by Pegler et al. (2014) and Zheng et al. (2015a).

Appropriate boundary and initial conditions are needed to complete the problem statement. We assume that fluid injection begins at \( t = 0 \) at the origin, and prior to that the
domain is filled with the resident (dense) fluid. The initial condition for Equation (2.6) is then given by

\[ h(r,0) = 0. \]  

(2.7)

The boundary condition at the front \( r = r_{N1}(t) \) of the interface requires

\[ h(r_{N1}(t),t) = 0. \]  

(2.8)

We can obtain a second boundary condition at \( r = 0 \), assuming the radius of the injection well is negligibly small. To do this, we first multiply \( r \) on both sides of Equation (2.6) and integrate from \( r = 0 \) to \( r = r_{N1}(t) \):

\[ \int_0^{r_{N1}(t)} r \frac{\partial h}{\partial t} \, dr = \frac{1}{\phi} \left[ \frac{\Delta \rho gkh(h_0 - h) r}{\mu_d h + \mu_i(h_0 - h)} \frac{\partial h}{\partial r} + \frac{q\mu_i(h_0 - h)}{2\pi(\mu_d h + \mu_i(h_0 - h))} \right]_{r=0}^{r_{N1}(t)}. \]  

(2.9)

Then, we multiply both sides of Equation (2.9) by \( 2\pi \phi \) and substitute in the global mass constraint (2.5). Also, we assume that there is no fluid entrainment at the front of the interface when we evaluate the term on the right hand side as \( r \to r_{N1}(t) \), i.e., \( h\frac{\partial h}{\partial r} \bigg|_{r \to r_{N1}(t)} = 0 \). Then, we obtain

\[ \left[ \frac{\Delta \rho gkh(h_0 - h) r}{\mu_d h + \mu_i(h_0 - h)} \frac{\partial h}{\partial r} + \frac{q\mu_i(h_0 - h)}{2\pi(\mu_d h + \mu_i(h_0 - h))} \right]_{r=0}^{r_{N1}(t)} = \frac{q}{2\pi}. \]  

(2.10)

The complete problem statement is then to solve Equation (2.6) subject to initial condition (2.7) and boundary conditions (2.8) and (2.10) and so obtain \( h(r,t) \) and the front location \( r_{N1}(t) \).
2.3.1 Non-dimensionalization

We can rescale Equation (2.6) by defining dimensionless variables $H \equiv h/h_0$, $R \equiv r/h_0$ and $T \equiv t/(2\pi h_0^3/q)$. Then, Equation (2.6) in dimensionless form is

$$\frac{\partial H}{\partial T} = \frac{1}{R} \frac{\partial}{\partial R} \left( \frac{\Gamma M H (1 - H) R \partial H}{1 + (M - 1) H} + \frac{1 - H}{1 + (M - 1) H} \right),$$

(2.11)

where $M$ and $\Gamma$ are two dimensionless groups defined as

$$M \equiv \frac{\mu_d}{\mu_i} \quad \text{and} \quad \Gamma \equiv \frac{2\pi \Delta \rho g k h_0^2}{\mu_d q}.$$

(2.12a, b)

By definition, $M$ is the viscosity ratio of the displaced fluid relative to the injected fluid, and $\Gamma$ measures the importance of buoyancy effects relative to fluid injection in driving the axisymmetric flow.

In addition, the dimensionless global mass conservation equation becomes

$$\int_{0}^{R_{N_1}(T)} RH(R,T) \, dR = T,$$

(2.13)

where $R_{N_1}(T) \equiv r_{N_1}(t)/h_0$ denotes the maximum radial extent of the front. The initial and boundary conditions can also be rewritten in dimensionless form:

$$H(R,0) = 0,$$

(2.14a)

$$H(R_{N_1}(T),T) = 0,$$

(2.14b)

$$\left. \left[ \frac{\Gamma M H (1 - H) R \partial H}{1 + (M - 1) H} + \frac{1 - H}{1 + (M - 1) H} \right] \right|_{R=0} = 1.$$

(2.14c)

Equation (2.11) with initial and boundary conditions (2.14) can be solved numerically to provide the time evolution of the fluid-fluid interface. We have implemented a central-difference scheme to solve this problem ([Kurganov and Tadmor, 2000; Zheng et al., 2015a], see also Appendix 2.A for more details. From the numerical results, we note that there may
Figure 2.2: Typical numerical solutions of the time evolution of the fluid-fluid interface, from solving Equation (2.11) subject to boundary and initial conditions (2.14), at different times $T = 1, 10$ for different values of $\Gamma$ and $M$. We chose $\Gamma = 1/10, 100$ and $M = 1/2, 1, 5$ to demonstrate the different types of solutions. (a), (c) and (e): $\Gamma = 1/10$ with $M = 1/2, 1, 5$, respectively. (b), (d) and (f): $\Gamma = 100$ with $M = 1/2, 1, 5$, respectively. The analytical solutions derived in Sections 2.4 and 2.5 are also shown: see Section 2.4.1 for (a), Section 2.4.2 for (c), Section 2.4.3 for (e), and Section 2.5 for (b), (d) and (f). Note that, for simplicity, black solid curves are used for analytical solutions at both $T = 1$ and $T = 10$ without confusion.
be a second radial location $R_{N2}(t) \equiv r_{N2}(t)/h_0$, where for all $R \leq R_{N2}(t)$, $H(R_{N2}(t)) = 1$ (see sketch in Figure 2.1). Typical numerical solutions are provided in Figure 2.2. The numerical solutions motivate us to seek different approximate solutions in asymptotic limits based on the two dimensionless groups $M$ and $\Gamma$, as defined in (2.12). We have also plotted in Figure 2.2 the analytical solutions we obtain in Sections 2.4 and 2.5, and we have observed very good agreement between the analytical and the numerical solutions. These approximate analytical solutions will be discussed more below. We note that the fluid-fluid interfaces in Figure 2.2(a) and (c) have a large slope, where the lubrication approximation can fail. Nevertheless, we will show (in Sections 2.4.1 and 2.4.2) that the slope decays with time as $1/\sqrt{T}$, so the lubrication approximation is valid at late times.

2.3.2 Similarity transform

Let us now define a similarity variable $\eta = R^2/T$. Then, Equation (2.11) can be rewritten in terms of $\eta$ only:

$$
\eta \frac{dH}{d\eta} + 2 \frac{d}{d\eta} \left( \frac{2\Gamma MH(1-H)\eta}{1+(M-1)H} \frac{dH}{d\eta} + \frac{1-H}{1+(M-1)H} \right) = 0.
$$

(2.15)

We can further obtain two boundary conditions at the propagating front $R_{N1}(T)$:

$$
H(\eta_{N1}) = 0,
$$

(2.16a)

$$
\left. \frac{dH}{d\eta} \right|_{\eta \to \eta_{N1}} = \frac{1}{2\eta_{N1}\Gamma} - \frac{1}{4\Gamma M},
$$

(2.16b)

where the constant $\eta_{N1} \equiv R^2_{N1}(T)/T$ represents the location of the propagating front in the $(\eta, H)$ space. From this point forward, whenever we use the term “front”, it means the frontal tips at the top or bottom boundaries. The boundary condition (2.16b) is derived by evaluating Equation (2.15) for $\eta \to \eta_{N1}$, where $H(\eta_{N1}) = 0$ (see Appendix 2.B for more details).
A shooting scheme is used to solve Equation (2.15) subject to boundary conditions (2.16a,b). In order to determine \( \eta_{N_1} \), an iterative procedure is needed, such that the global mass conservation condition is satisfied:

\[
\int_0^{\eta_{N_1}} H(\eta) \, d\eta = 2. \tag{2.17}
\]

As mentioned in Section 2.3.1, the fluid-fluid interface may intersect with both boundaries, and contains a fast front \( R_{N_1}(T) \) with \( H(R_{N_1}(T), T) = 0 \) and a slow front \( R_{N_2}(T) \) with \( H(R_{N_1}(T), T) = 1 \) (see sketch in Figure 2.1 and numerical results in Figure 2.2). Equivalently, the numerical shooting procedure here may generate a second front in the \((\eta, H)\) space, which corresponds to \( \eta_{N_2} = R_{N_2}^2/T \) with \( H(\eta_{N_2}) = 1 \). The initial condition is not necessary since we are looking for a self-similar solution, which represents the intermediate asymptotic behavior with the initial condition eventually forgotten (Barenblatt, 1979).

We note that Equation (2.15) is analogous to Equation (11) in the paper of Nordbotten and Celia (2006). In addition, for the limit of \( \Gamma \ll 1 \), i.e., when fluid injection effect is much more important than buoyancy effect in driving the fluid flow, by neglecting the second-order term in Equation (2.15), Nordbotten and Celia (2006) obtained a rarefaction wave solution for \( M > 1 \). In this chapter, we provide two additional approximate solutions in Section 2.4 for \( M = 1 \) and \( M < 1 \), respectively, when the flow is mainly driven by injection \( (\Gamma \ll 1) \). In Section 2.5 we show that when \( \Gamma \gg 1 \), i.e., when the flow is mainly driven by buoyancy, for the majority part of the fluid-fluid interface away from the narrow region near the injection site, the well-known nonlinear diffusion equation that describes the propagation of a gravity current in an unconfined porous medium can be used to describe the flow behavior (see, e.g., Lyle et al., 2005). We also numerically calculate the boundaries when each analytical approximation provides good estimates, and summarize the flow behaviors in a \( \Gamma-M \) regime diagram in Section 2.6.
2.4 Injection-driven regimes: $\Gamma \ll 1$

When $\Gamma \ll 1$, the fluid flow is mainly driven by injection. In this case, the flow is confined, and the fluid-fluid interface intersects with both the top and bottom boundaries. In Sections 2.4.1 to 2.4.3, we present three analytical solutions for $M < 1$, $M = 1$, and $M > 1$, respectively, in the limit of $\Gamma \ll 1$. Physically, these three approximate solutions correspond to the injection-driven flows with less viscous, equally viscous, and more viscous displaced fluids, respectively, compared with the injected fluid.

2.4.1 Less viscous displaced fluid: $M < 1$

When $M < 1$, the injected fluid is more viscous than the displaced fluid. When $\Gamma \ll 1$, numerical simulations of Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17) indicate that the fluid-fluid interface in the $(\eta, H)$ space appears as a straight line with a slope depending on the value of $M$. We first note that if the fluid-fluid interface propagates as a shock (vertical interface), the interface location corresponds to $\eta = 2$ in the $(\eta, H)$ space, according to the global mass constraint (2.17). Motivated by the numerical observation, we now define a new variable $\zeta \equiv (\eta - 2)/\Gamma \alpha$, substitute it into Equation (2.15), and we obtain

$$
(\Gamma^\alpha \zeta + 2) \frac{dH}{d\zeta} + 2 d \frac{d}{d\zeta} \left( \frac{2M(\Gamma^\alpha \zeta + 2)\Gamma^{1-\alpha}H(1-H)}{1+(M-1)H} \frac{dH}{d\zeta} + \frac{1-H}{1+(M-1)H} \right) = 0. \tag{2.18}
$$

To balance the terms associated with diffusion and advection, i.e., the two terms within the bracket of the differentiation in (2.18), we need $\alpha = 1$. Neglecting the $O(\Gamma)$ terms in Equation (2.18), we obtain

$$
\frac{dH}{d\zeta} + d \frac{d}{d\zeta} \left( \frac{4MH(1-H)}{1+(M-1)H} \frac{dH}{d\zeta} + \frac{1-H}{1+(M-1)H} \right) = 0. \tag{2.19}
$$
Since the flow is confined, we have two front conditions:

\[ H(\zeta_{N_1}) = 0, \quad \text{and} \quad H(\zeta_{N_2}) = 1, \quad (2.20a,b) \]

where \( \zeta_{N_1} \equiv (\eta_{N_1} - 2)/\Gamma \) and \( \zeta_{N_2} \equiv (\eta_{N_2} - 2)/\Gamma \equiv (R_{N_2}^2(T)/T - 2)/\Gamma \), which refer to the intersections with the top and bottom boundaries, respectively (e.g., see Figure 2.1). The global mass conservation Equation (2.17) in this case can be rewritten as

\[ \zeta_{N_2} + \int_{\zeta_{N_1}}^{\zeta_{N_2}} H(\zeta) \, d\zeta = 0. \quad (2.21) \]

We first integrate Equation (2.19) once and obtain:

\[ H + \frac{4MH(1-H)}{1+(M-1)H} \frac{dH}{d\zeta} + \frac{1-H}{1+(M-1)H} = 1, \quad (2.22) \]

where the integration constant is obtained from the front conditions (2.20). Equation (2.22) can be reorganized as

\[ (1-H)H \left( \frac{dH}{d\zeta} - \frac{M-1}{4M} \right) = 0, \quad (2.23) \]

which immediately suggests that \( H = 0, H = 1, \) or \( H \) has a linear structure:

\[ \frac{dH}{d\zeta} = \frac{M-1}{4M}. \quad (2.24) \]

Integrating Equation (2.24) once more, we obtain

\[ H(\zeta) = \frac{(M-1)}{4M} \zeta + \frac{1}{2}, \quad (2.25) \]
Figure 2.3: A comparison of the numerical solutions of Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17) and the analytical solution (2.28) for $\Gamma = 0.01, 0.05, 0.1$ and $M = 1/2$. (a) $H$ as a function of $\eta = R^2/T$. Note that, for simplicity, black solid lines are used for analytical solutions for all $\Gamma$ values without confusion. (b) $H$ as a function of the rescaled variable $\zeta \equiv (R^2/T - 2)/\Gamma$.

where the integration constant is chosen such that the global mass conservation Equation (2.21) is satisfied. The locations of the two fronts are also determined:

$$\zeta_{N1} = \frac{2M}{1-M} \quad \text{and} \quad \zeta_{N2} = -\frac{2M}{1-M},$$

(2.26a,b)

or equivalently,

$$\eta_{N1} = 2 + \frac{2M}{1-M} \Gamma \quad \text{and} \quad \eta_{N2} = 2 - \frac{2M}{1-M} \Gamma.$$

(2.27a,b)
Thus, we have obtained an approximate solution for $M < 1$ and $\Gamma \ll 1$:

$$H(\eta) = \begin{cases} 
1, & 0 \leq \eta \leq 2 - \frac{2M}{1-M} \Gamma; \\
\frac{M-1}{4M} (\eta - 2) + \frac{1}{2}, & 2 - \frac{2M}{1-M} \Gamma < \eta \leq 2 + \frac{2M}{1-M} \Gamma; \\
0, & \eta > 2 + \frac{2M}{1-M} \Gamma.
\end{cases} \tag{2.28}$$

The fluid-fluid interface has a linear structure in the $(\eta, H)$ space and a parabolic structure in the $(R, H)$ space for a fixed time $T$. We note that the slope of the fluid-fluid interface is constant in the $(\eta, H)$ space and decays with time as $1/\sqrt{T}$ in the $(R, H)$ space, which supports the lubrication approximation at late times. To verify this solution, we numerically solve Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17), and we compare this numerical solution with the analytical solution (2.28). The comparison is plotted in Figure 2.3 with $M = 1/2$ and $\Gamma = 0.01, 0.05, 0.1$ as examples, and we have observed very good agreement.

### 2.4.2 Equally viscous displaced fluid: $M = 1$

When $M = 1$, the injected and displaced fluids are equally viscous. Again, we note that if the fluid-fluid interface propagates as a vertical interface (shock), the location of this interface corresponds to $\eta = 2$ in the $(\eta, H)$ space, according to the global mass constraint (2.17). Motivated by our numerical results, we now define $\zeta_e \equiv (\eta - 2)/\Gamma^\beta$ and substitute it into Equation (2.15) with $M = 1$ to obtain

$$\zeta_e \Gamma^\beta \frac{dH}{d\zeta_e} + 4 \frac{d}{d\zeta_e} \left( \Gamma^{-1/\beta} (1 - H) H \left( \Gamma^\beta \zeta_e + 2 \right) \frac{dH}{d\zeta_e} \right) = 0. \tag{2.29}$$

The first term in (2.29) corresponds to both the unsteady and advective terms in the partial differential Equation (2.11), while the second term is related to the diffusive term in (2.11). We note that, when $\Gamma \ll 1$, $\beta = 1/2$ is required for a balance of the advective and diffusive
terms. Then we obtain

\[ \zeta_e \frac{dH}{d\zeta_e} + 4 \frac{d}{d\zeta_e} \left( (1 - H)H \left( \Gamma^{1/2} \zeta_e + 2 \right) \frac{dH}{d\zeta_e} \right) = 0. \]  

(2.30)

Next, we neglect the \( O(\Gamma^{1/2}) \) terms in (2.30) and obtain

\[ \zeta_e \frac{dH}{d\zeta_e} + 8 \frac{d}{d\zeta_e} \left( (1 - H)H \frac{dH}{d\zeta_e} \right) = 0. \]  

(2.31)

The front conditions are analogous to (2.20):

\[ H \left( \zeta_{eN_1} \right) = 0, \quad H \left( \zeta_{eN_2} \right) = 1, \]  

(2.32a, b)

with \( \zeta_{eN_1} \equiv (\eta_{N_1} - 2)/\Gamma^{1/2} \) and \( \zeta_{eN_2} \equiv (\eta_{N_2} - 2)/\Gamma^{1/2} \) representing the locations of the fast and slow fronts. The global mass conservation Equation (2.17) has the same form as (2.21):

\[ \zeta_{eN_2} + \int_{\zeta_{eN_1}}^{\zeta_{eN_2}} H(\zeta_e) \, d\zeta_e = 0. \]  

(2.33)

Equation (2.31) has an analytical solution, which satisfies both the front conditions (2.32) and the global mass conservation Equation (2.33):

\[ H = -\frac{1}{4} \zeta_e + \frac{1}{2}. \]  

(2.34)

The locations of the fronts are also determined from (2.32) and (2.34):

\[ \zeta_{eN_1} = 2 \quad \text{and} \quad \zeta_{eN_2} = -2, \]  

(2.35a, b)

or equivalently,

\[ \eta_{N_1} = 2 + 2\sqrt{\Gamma} \quad \text{and} \quad \eta_{N_2} = 2 - 2\sqrt{\Gamma}. \]  

(2.36a, b)
To summarize, we have obtained an approximate solution for $M = 1$ and $\Gamma \ll 1$:

$$H(\eta) = \begin{cases} 
1, & 0 \leq \eta \leq 2 - 2\sqrt{\Gamma}; \\
-\frac{1}{4} \frac{\eta - 2}{\sqrt{\Gamma}} + \frac{1}{2}, & 2 - 2\sqrt{\Gamma} < \eta \leq 2 + 2\sqrt{\Gamma}; \\
0, & \eta > 2 + 2\sqrt{\Gamma}. 
\end{cases}$$

(2.37)

Solution (2.37) displays a very good agreement with the numerical solution to Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17) with $\Gamma \ll 1$ and $M = 1$, as shown in Figure 2.4. We have chosen $\Gamma = 0.01, 0.05, 0.1$ as exam-
Figure 2.5: A comparison of the numerical solutions of Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17) and the analytical solution (2.40) for $\Gamma = 0.01, 0.05, 0.1$ and $M = 5$.

The fluid-fluid interface has a linear structure in the $(\eta, H)$ space and a parabolic shape in the $(R, H)$ space for a fixed time $T$. The slope of the fluid-fluid interface decays with time as $1/\sqrt{T}$ in the $(R, H)$ space, thus, the validity of the lubrication approximation is supported at late times.

### 2.4.3 More viscous displaced fluid: $M > 1$

When $M > 1$, the displaced fluid is more viscous than the injected fluid. Similar to the analogous problem in Cartesian geometries (Pegler et al., 2014; Zheng et al., 2015a), when $\Gamma \ll 1$, we neglect the second-order derivative term in Equation (2.15) that is associated with buoyancy. Then, Equation (2.15) is reduced to

$$
\eta \frac{dH}{d\eta} + 2 \frac{d}{d\eta} \left( \frac{1 - H}{1 + (M - 1)H} \right) = 0.
$$

(2.38)

The solution to (2.38) should satisfy both the global mass constraint (2.17) and the front conditions:

$$
H(\eta_N_1) = 0, \quad H(\eta_N_2) = 1.
$$

(2.39a, b)
We can obtain an analytical solution (a rarefaction solution):

\[
H(\eta) = \begin{cases} 
1, & 0 \leq \eta \leq 2/M; \\
\left(\sqrt{2M/\eta} - 1\right)/(M - 1), & 2/M < \eta \leq 2M; \\
0, & \eta > 2M,
\end{cases}
\]

which has been reported previously citepnordbotten2006similarity, and the locations of the fronts are

\[
\eta_{N_1} = 2M, \quad \eta_{N_2} = 2/M. \tag{2.41a,b}
\]

We can compare the rarefaction solution (2.40) with the numerical solution to Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17). We observe good agreement when \( \Gamma \) is small, as shown in Figure 2.5 with \( \Gamma = 0.01, 0.05, 0.1 \) and \( M = 5 \) as examples. In addition, the most significant deviation is found near the bottom boundary, where the buoyancy effect is the strongest along the fluid-fluid interface. Similar behaviors have also been reported in the analogous problem in Cartesian coordinates (Pegler et al. 2014; Zheng et al., 2015a).

### 2.5 Buoyancy-driven regime: \( \Gamma \gg 1 \)

When \( \Gamma \gg 1 \), numerical simulation indicates that for the majority part of the interface (except the narrow region near the origin), the thickness of the interface is small compared with the thickness of the porous medium (see, e.g., Figure 2.2b,d,f). Thus, the flow is mainly unconfined, buoyancy is the main driving force for the propagation of the injected fluid, and we neglect the advective term in Equation (2.11) that is associated with fluid injection. In addition, since the thickness is small, both \( H \ll 1 \) and \( |(M - 1)H| \ll 1 \) hold.
Figure 2.6: A comparison of the solution to Equation (2.15) subject to boundary conditions (2.16) and global mass constraint (2.17) and the solution to (2.44) subject to (2.45). (a) $H$ as a function of $R^2/T$. Note that, for simplicity, black solid curves are used for analytical solutions for all $\Gamma$ values without confusion. (b) $f \equiv \Gamma M H / \eta N_1$ as a function of $y \equiv \eta / \eta_{N_1}$. We have chosen $\Gamma = 10, 100, 500$ and $M = 1$ as examples.

for the majority part of the interface. Then, Equation (2.11) reduces to:

$$\frac{\partial H}{\partial T} = \frac{\Gamma M}{R} \frac{\partial}{\partial R} \left( R H \frac{\partial H}{\partial R} \right),$$

which is the well-known nonlinear diffusion equation for the propagation of a gravity current in an unconfined porous medium (see, e.g., [Bear 1972, Lyle et al. 2005]). Together with the global mass conservation Equation (2.5), a self-similar solution can be obtained for the time evolution of the fluid-fluid interface that is away from the narrow region near the injection site.
As discussed in Section 2.3, we define the similarity variable as $\eta \equiv R^2/T$. Then, Equation (2.42) can be transformed to

$$\eta \frac{dH}{d\eta} + 4\Gamma M \frac{d}{d\eta} \left( \eta H \frac{dH}{d\eta} \right) = 0. \quad (2.43)$$

Note that Equation (2.43) can also be derived from Equation (2.15). We further define $y \equiv \eta/\eta_1$ and $f \equiv \Gamma MH/\eta_1$. Then, Equation (2.42) can be rewritten as

$$4 (yf')' + yf'' = 0. \quad (2.44)$$

Two boundary conditions are needed to solve (2.44), which can be derived from Equation (2.16a,b):

$$f|_{y \to 1^-} = 0, \quad (2.45a)$$

$$f'|_{y \to 1^-} = -1/4. \quad (2.45b)$$

In addition, the global mass conservation Equation (2.13) can be used to calculate the location of the fast front $\eta_1$:

$$\eta_1 = \left( 2\Gamma M \int_0^1 f(y)dy \right)^{1/2}. \quad (2.46)$$

Note that we have neglected the influence of the slow front along the bottom boundary since it is very close to the origin, and the effect on the location of the fast front is negligibly small. For more details about this approximation, see Appendix 2.C.

Equation (2.44) can be solved numerically with boundary conditions (2.45a,b), which is shown in Figure 2.6b; then, Equation (2.46) can be used to find the location of the front $\eta_1$, which intersects with the top boundary. We can also solve the nonlinear advection-diffusion Equation (2.15) numerically subject to boundary conditions (2.16) and global...
mass constraint (2.17). A comparison of this numerical solution and the self-similar solution by solving Equation (2.44) with \((2.45a, b)\) are provided in Figure 2.6. We observe very good agreement between the solutions for large values of \(\Gamma\), which confirms that for the majority part of the fluid-fluid interface that is away from the injection site, the effect of the slow front is negligible, and the assumption of unconfined flows is appropriate.

### 2.6 Injection regimes

#### 2.6.1 Injection regimes

Five distinct self-similar flow regimes have been identified and summarized in a phase-type diagram, as shown in Figure 2.7 with respect to two dimensionless groups \(\Gamma\) and \(M\). Recall that \(M\) denotes the viscosity ratio of the displaced to the injected fluids, and \(\Gamma\) measures the importance of buoyancy relative to fluid injection effects. The five regimes include four regimes representing the different asymptotic limits and an intermediate regime. The boundaries between each individual regime are calculated based on a 10% difference of the top front location between the prediction of each asymptotic solution and the prediction of the direct numerical solution to Equation (2.15), as discussed in Section 2.3. The five individual flow regimes are:

- **Regime I** \((\Gamma \ll 1 \text{ and } M < 1)\): the axisymmetric flow is mainly driven by fluid injection with the injected fluid being more viscous than the displaced fluid. A new approximate solution (2.28) is identified in this regime, which represents a parabolic shape for the fluid-fluid interface, as discussed in Section 2.4.1. The interface intersects with both the top and bottom boundaries, and the intersections represent the horizontal extent of the interface.

- **Regime II** \((\Gamma \ll 1 \text{ and } M = 1)\): the flow is mainly driven by fluid injection with the injected and displaced fluids having the same viscosity. Another new approximate
Figure 2.7: Regime diagram for the axisymmetric flows generated by fluid injection into a horizontal confined porous medium initially saturated with another immiscible fluid of different density and viscosity. Five distinct self-similar regimes, summarized in Section 2.6.1, are identified based on two dimensionless control parameters: $\Gamma$, representing the relative importance of buoyancy effect over injection effect, and $M$, the viscosity ratio of the displaced to the injected fluids. In regime I, an approximate analytical solution (2.28) is obtained that indicates a parabolic interface shape. In regime II, a distinct approximate analytical solution (2.37) is obtained to characterize the parabolic interface shape. In regime III, a rarefaction solution (2.40) is obtained to describe the dynamics of the fluid-fluid interface that attaches to both boundaries. In regime IV, buoyancy is the major driving force, the majority of the fluid-fluid interface away from the injection point is unconfined with a well-known self-similar solution (Section 2.5). There is an intermediate regime V that describes the flow behavior when both injection and buoyancy effects are important. More discussions on the regime boundaries (the dashed curves) are provided in Section 2.6.2.
analytical solution (2.37) is obtained in this regime, as discussed in Section 2.4.2. Solution (2.37) represents a parabolic shape for the fluid-fluid interface, which contains intersections with both the top and bottom boundaries.

- Regime III ($\Gamma \ll 1$ and $M > 1$): the flow is mainly driven by fluid injection with the injected fluid less viscous than the displaced fluid. A rarefaction solution (2.40) can be used to describe the dynamics of the interface shape (Nordbotten and Celia, 2006), as discussed in Section 2.4. The rarefaction solution (2.40) also predicts intersections with both the top and bottom boundaries.

- Regime IV ($\Gamma \gg 1$): the flow is mainly buoyancy-driven. For the majority part of the interface (except the region close to the origin), the interface is far away from the bottom boundary, and the governing Equation (2.11) for the fluid-fluid interface reduces to the well-known nonlinear diffusion Equation (2.42) that describes the spreading of gravity currents in an unconfined porous medium. A self-similar solution can be obtained that is independent of the value of the viscosity ratio $M$ (Lyle et al., 2005), as discussed in Section 2.5.

- Regime V: This regime is intermediate between each of the individual asymptotic limits, and the axisymmetric flow is due to both injection and buoyancy effects. Direct numerical simulation of Equation (2.15) is necessary to obtain the time evolution of the fluid-fluid interface, and the location of the propagating fronts.

2.6.2 Regime boundaries

The regime boundary $M = 1$ is obvious, with $M$ representing the viscosity ratio of the displaced to the injected fluids. We now explain the asymptotic behavior of the regime boundaries using scaling arguments:

- $M \ll 1$ and $\Gamma \gg 1$: Numerical observation indicates that the boundary of Regimes IV and V has a slope of $-1$ when $M \ll 1$ in the log-log plot of $\Gamma$ versus $M$. This slope
is related to the condition $H \ll 1$ as $M \ll 1$, under which the confinement effect is negligible for the majority part of the interface away from origin, and Equation (2.11) reduces to (2.42), as discussed in Section 2.5. Since $H \approx (\Gamma M)^{-1/2}$ in Regime IV, as an *a priori* estimate, we obtain a crossover condition $(\Gamma M)^{-1/2} \approx 1$, which indicates a slope of $-1$ for the regime boundary.

- $M \gg 1$ and $\Gamma \gg 1$: From numerical simulation, the boundary of Regimes IV and V has a slope of 1 when $M \gg 1$ in the log-log plot of $\Gamma$ versus $M$. This behavior is associated with the condition $|(M-1)H| \ll 1$ as $M \gg 1$, under which Equation (2.11) reduces to (2.42), as discussed in Section 2.5. Again, since $H \approx (\Gamma M)^{-1/2}$ in Regime IV, as an *a priori* estimate, we obtain the crossover condition $(\Gamma/M)^{-1/2} \approx 1$, which indicates a slope of 1 for the regime boundary.

- $M \gg 1$ and $\Gamma \ll 1$: The boundary between Regimes III and V is related to the condition under which Equation (2.15) reduces to (2.38), i.e.,

$$\frac{d}{d\eta} \left( \frac{2\Gamma MH(1-H)\eta dH}{1+(M-1)H} \right) / \frac{d}{d\eta} \left( \frac{1-H}{1+(M-1)H} \right) \ll 1,$$

(2.47)

As an *a priori* estimate, we substitute solution (2.40) into (2.47), and, after some algebra, we obtain $\Gamma/(M-1) \ll 1$. Thus, the crossover condition $\Gamma/(M-1) \approx 1$ can be used to describe the qualitative behavior of this regime boundary. In particular, for $M \gg 1$, we obtain $\Gamma/M \approx 1$, which represents a slope of 1 in the log-log plot of $\Gamma$ versus $M$, and this slope agrees with the numerical observation; for $M \to 1^+$, $\Gamma/(M-1) \approx 1$ indicates a singular behavior that also appears in our numerical simulations.

- $M \ll 1$ and $\Gamma \ll 1$: The boundary between Regimes I and V is related to the emergence of the slow front along the bottom boundary, i.e., $2 - 2M\Gamma/(1 - M) > 0$. The qualitative behavior of the regime boundary is related to the crossover condition $2 - 2M\Gamma/(1 - M) = 0$. For $M \ll 1$, this crossover condition reduces to $M\Gamma \approx 1$, 39
which indicates a slope of $-1$ in the log-log plot of $\Gamma$ versus $M$; for $M \to 1^-$, we obtain $\Gamma/(1 - M) \approx 1$, which indicates a singular behavior. Both predictions as $M \ll 1$ and $M \to 1^-$ have been observed in our numerical simulations.

## 2.7 Transition to self-similar solutions

Given an initial condition, in general, there exists a transition time period for the self-similar solutions to be fully developed, since the self-similar solutions do not contain information of the initial condition. The approximate analytical solutions we obtained in Sections 2.4...
and 2.5, and summarized in the regime diagram Figure 2.7, are all self-similar solutions that hold after the initial transition period. To study this transition behavior from an initial condition to a self-similar solution, we numerically solve the partial differential Equation (2.11), subject to initial and boundary conditions (2.14), and obtain the time evolution of the front locations and the shape of the fluid-fluid interface over a wide range of time scales for different values of $M$ and $\Gamma$. Then, for both the time evolution of the front locations and the fluid-fluid interface, we compare the predictions from the numerical solutions with those from the self-similar solutions we obtained in Sections 2.4 and 2.5.

2.7.1 Location of the propagating fronts

The propagation laws of the fast ($R_{N_1}$) and slow ($R_{N_2}$) fronts are shown in Figures 2.8a and 2.8b, respectively, for a wide range of time $T$ and representative values of $\Gamma$ and $M$. The predictions from various self-similar solutions are shown as the dashed lines, while the numerical results are plotted as the symbols. The $T^{1/2}$ power-law behavior for the propagating fronts has been observed from the numerical results. Within the time range we considered, the self-similar solutions provide very good approximations for the location of both the fast and slow fronts.

2.7.2 Shape of the fluid-fluid interface

We show in this section the transition behavior of the fluid-fluid interface. In particular, in Figure 2.9, we show the interface shapes in the $(\eta, H)$ space at $T = \{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^0, 10^1\}$ for different representative values of $M$ and $\Gamma$. We have chosen $\Gamma = 0.1$ for Regime I to III, i.e., the injection-driven regimes, and $\Gamma = 100$ for the buoyancy-driven Regime IV. Within the time range we consider, very good agreements have been observed between the predictions of the numerical results and the self-similar solutions.

In addition, within this time range, we observe that the numerical curves for the interface shape collapse to each other, i.e., the transition process to develop the self-similar so-
Figure 2.9: Time evolution of the shape of the fluid-fluid interface in the $(\eta, H)$ space at $T = \{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^0, 10^1\}$. The solid curves are generated from numerically solving the partial differential Equation (2.11), subject to initial and boundary conditions (2.14). The dashed curves are from the approximate analytical solutions we obtained in Sections 2.4 and 2.5. We have chosen $\Gamma = 0.1$ as an example to demonstrate the flow behaviors in Regime I to III, the injection-driven regimes, and $\Gamma = 100$ as an example for the buoyancy-driven Regime IV.

Solutions is not obvious in our numerical simulation. We note that $T \to 0^+$ maps to $\eta \to +\infty$ by definition, and from boundary condition (2.16a) we have $H(+\infty) = 0$. Thus, the initial condition (2.14a), i.e., $H(X, 0) = 0$, is in the solution space of the self-similar solution of Equation (2.15). The global mass constraint (2.13) is also satisfied by $H(X, 0) = 0$ as $T \to 0^+$. Therefore, the similarity solution to ordinary differential equation (ODE) (2.15) is an exact solution (for all time) to partial differential equation (PDE) (2.11), subject to boundary and initial conditions (2.14), and no transition period is necessary to develop the appropriate analytical solutions (self-similar solutions) we obtained in Sections 2.4 and 2.5, and these solutions hold from $T = 0$. 

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Table 2.2: Examples of practical fluid injection projects, including CO\textsubscript{2}-WAG enhanced oil recovery (EOR, case 1), geological CO\textsubscript{2} storage (cases 2 and 3), and underground waste disposal (case 4). The value of the dimensionless groups $M$ and $\Gamma$ are calculated based on (2.12), and indicates the behavior of the axisymmetric flows and the corresponding approximate solutions.

2.8 Practical implications

We briefly discuss the practical implications of the approximate analytical solutions, as summarized in the self-similar regime diagram (Figure 2.7) in this section. We consider different engineering applications such as enhanced oil recovery, geological CO\textsubscript{2} sequestration, and underground waste disposal projects. We note that the axisymmetric assumption holds for horizontal geological formations. It has also been shown to be a good assumption for inclined formations with a slope up to 1°, as long as the force from injection is the dominant driving force (Gasda et al., 2008). The dimensional physical properties and the value for the dimensionless parameters ($\Gamma$ and $M$) we calculated based on (2.12) for each individual project are listed in table 2.2.

- Case 1: The first example comes from a large-scale CO\textsubscript{2}-WAG (Water-alternating-gas) enhanced oil recovery project at the Kelly-Snyder oil fields in Texas (see, e.g.,
The values of the dimensionless control parameters are $\Gamma \approx 0.26$ and $M \approx 0.14$, where the $\Gamma$ value is calculated with the density difference between water and CO$_2$ (324 kg/m$^3$). Thus, the axisymmetric flow, for example, from water injection (displacing CO$_2$ that was previously injected into the reservoir) in this project lies in Regime I, and the approximate analytical solution (2.28) can be used to characterize the time evolution of the interface between water and CO$_2$. We recognize that the CO$_2$-WAG process is complicated as it involves multiple interfaces between different fluids (water-CO$_2$, CO$_2$-oil). Here, we only focus on the water-CO$_2$ interface that is formed when water displaces the previously injected CO$_2$. We also note that this case has a more dense injected fluid (water) displacing a less dense fluid (CO$_2$), where the fluid-fluid interface should be flipped upside down compared to that of a less dense fluid displacing a more dense fluid (see Figure 2.1).

- Case 2: The second example is the world’s first and longest running industrial-scale geological CO$_2$ sequestration project in a saline aquifer at Sleipner in the North Sea (see, e.g., [Singh et al., 2010]). The target formation for CO$_2$ storage at the Sleipner site has very high permeability in a range from $1 \times 10^{-12}$ m$^2$ to $5 \times 10^{-12}$ m$^2$. This formation contains a number of thin intra-formational shale layers (approximately 0.5 to 2 m thick) that separate the formation into nine sand layers. Most of the modeling efforts in the literature focused on the ninth sand layer (the uppermost layer) because this layer has the most available geophysical data. In addition, this layer is relatively homogeneous (permeability: $\approx 2 \times 10^{-12}$ m$^2$), and it has been shown that the vertical equilibrium models are applicable (see, e.g., [Nilsen et al., 2011]). The representative values of the related parameters in table 2.2 are taken from the 2010 benchmark problem ([Singh et al., 2010]). The mass rate of CO$_2$ “injection” into the upper-most layer is reported to have increased from 0.02 Mt/year in 1999 to 1.56 Mt/year in 2009 ([Singh et al., 2010]). Here we consider the CO$_2$ flow behavior from 2005 to 2009 when the mass rate was between around 0.5 Mt/year and 1.56 Mt/year.
and use an average mass rate of 1 Mt/year to calculate the $\Gamma$ value. The values of the dimensionless control parameters are $\Gamma \approx 0.4$ and $M \approx 13$. Our calculation indicates that the flow behavior in the Sleipner project lies in Regime V. Therefore, the rarefaction wave solution (2.40) can be used to characterize the propagation of the interface between supercritical CO$_2$ and brine that originally saturates the aquifer.

- **Case 3:** We now consider the early year 1999, when the injection rate is reported to be around 0.02 Mt/year. The values of the control parameters are $\Gamma \approx 20$ and $M \approx 13$. Thus, the flow behavior lies in Regime IV, and buoyancy is the major driving force for the spreading of the supercritical CO$_2$. The well-known self-similar solution to the nonlinear diffusion Equation (2.44) can be used to describe the propagation of the CO$_2$-brine interface, as discussed in Section 2.5.

- **Case 4:** The fourth example is an underground liquid waste disposal project in a saline aquifer (see, e.g., Ortoleva and Liu, 1995). The values of the dimensionless control parameters are $\Gamma \approx 0.02$ and $M \approx 1.3$. Thus, the axisymmetric flow in this project lies in Regime III, and the rarefaction solution (2.40) can be used to characterize the time evolution of the shape of the interface between the injected liquid waste and brine that originally saturates the formation.

### 2.9 Final remarks

#### 2.9.1 Summary of major findings

Motivated by underground fluid injection processes through vertical wells, we study the axisymmetric flows generated from fluid injection into a horizontal confined porous medium that is originally saturated with another fluid of different density and viscosity. We have obtained a nonlinear advection-diffusion equation to describe the time evolution of the fluid-fluid interface by neglecting the effects of fluid mixing and interfacial tension. Two
dimensionless groups are identified which control the fluid flow: $M$, the viscosity ratio of the displaced fluid over the injected fluid, and $\Gamma$, the relative importance of buoyancy effect compared to fluid injection effect. We have obtained four approximate analytical solutions (self-similar solutions) in asymptotic limits involving $\Gamma$ and $M$: (i) an analytical solution (2.28) that indicates a parabolic interface shape for the injection-driven flow with a more viscous injected fluid than the displaced fluid (Regime I, $\Gamma \ll 1$ and $M < 1$); (ii) an analytical solution (2.37) that describes the injection-driven flow with equally viscous injected and displaced fluids (Regime II, $\Gamma \ll 1$ and $M = 1$); (iii) a rarefaction solution (2.40) that describes the injection-driven flow with a less viscous injected fluid than the displaced fluid (Regime III, $\Gamma \ll 1$ and $M > 1$); and (iv) the well-known self-similar solution that characterizes the buoyancy-driven flow in an unconfined porous medium (Regime IV, $\Gamma \gg 1$). We have obtained a regime diagram (Figure 2.7) to summarize the various flow behaviors. The regime diagram includes five distinct self-similar behaviors: the four asymptotic regimes and an intermediate regime. We have also briefly discussed the implications of the approximate analytical solutions and the regime diagram to practical projects such as enhanced oil recovery, geological CO$_2$ sequestration, and underground waste disposal projects.

2.9.2 Vertical equilibrium assumption and lubrication approximation

This validity of the nonlinear Equation (2.11) relies on two assumptions. First, the vertical equilibrium assumption indicates that the injected and displaced fluids are segregated due to strong buoyancy effects and form a sharp interface, i.e., the time scale we consider is larger than the time scale for the two fluids to segregate. Second, the assumption of the lubrication approximation requires that the gravity current is long and thin (the ratio of the height relative to length is small) and the slope of the fluid-fluid interface is small ($|\partial H / \partial R| \ll 1$). These two assumptions should be satisfied for the results in this chapter to be applicable.
The vertical equilibrium assumption is considered reasonable and has been verified using full multidimensional models in the context of geological CO\textsubscript{2} sequestration (see, e.g., Nordbotten and Dahle, 2011; Court et al., 2012; Guo et al., 2014a). Detailed discussions on the validity of the vertical equilibrium assumption can also be found in other references (see, e.g., Lake, 1989; Yortsos, 1995). In our study, the slope of the fluid-fluid interface decays with time as $1/\sqrt{T}$, as predicted from the self-similar solutions; thus, the validity of the lubrication approximation assumption is supported at late times. We also note that the slope of the fluid-fluid interface can be large in the region very close to the injection point (e.g., in regime IV); nevertheless, the self-similar solution successfully describes the bulk part of the fluid-fluid interface and the location of the propagating front, which is verified by laboratory experiments (see, e.g., Lyle et al., 2005).

### 2.9.3 Saffman-Taylor instability

We note that when the injected fluid is less viscous than the displaced fluid ($M > 1$), the flow situation corresponds to the condition when the Saffman-Taylor instability occurs (see, e.g., Saffman and Taylor, 1958; Homsy, 1987). In the injection dominant regime (Regime III), we obtained a rarefaction solution, which was previously studied by Nordbotten and Celia (2006). Similar behavior has also been identified for the analogous problem in Cartesian coordinates for fluid injection through a horizontal well into a confined porous medium initially saturated with another fluid of different density and larger viscosity (Pegler et al., 2014; Zheng et al., 2015a). Experiments have been conducted in Hele-Shaw cells filled with glass beads in Pegler et al. (2014), and it was observed that the Saffman-Taylor instability does not occur at the length scale of the Hele-Shaw cells. Within the time scale of the experiment, the theoretical predictions provide good approximations except in the region close to the propagating front. The suppression of the Saffman-Taylor instability is likely due to the inherent buoyant segregation in the system (Pegler et al., 2014).
2.A Appendix: Numerical simulations

We solve the nonlinear advection-diffusion Equation (2.11) numerically on a fixed domain \((0, L)\), instead of simulating the moving boundary problem on \((0, R_{N_1}(T))\) (see, e.g., Zheng et al., 2014, 2015a). The appropriate boundary conditions are provided at \(R = 0\) and \(R = L\). Since fluid injection begins at \(T = 0\), and we assume that there is only displaced fluid in the porous medium before injection; therefore, the initial condition is given by

\[
H(R, 0) = 0. \quad (2.48)
\]

Note that \(H(R, T) = 0\) holds ahead of the front, i.e., \(R \geq R_{N_1}(T)\); thus, the boundary condition at \(R = L\) is given by

\[
H(L, T) = 0. \quad (2.49)
\]

We multiply \(R\) to both sides of Equation (2.11), integrate it from \(R = 0\) to \(R = L\), and we obtain

\[
\frac{d}{dT} \int_0^L R \, dR + \left[ \Gamma M H (1 - H) R \frac{\partial H}{\partial R} + \frac{1 - H}{1 + (M - 1) H} \right]_0^L = 0. \quad (2.50)
\]

We consider constant fluid injection in this chapter, which gives \(\int_0^L R \, dR = T\). Then, employing Equation (2.49) and \(\lim_{R \to L} H \frac{\partial H}{\partial R} = 0\), i.e., no fluid entrainment at the front, Equation (2.50) can be rewritten to provide a boundary condition at \(R = 0\):

\[
\left[ \Gamma M H (1 - H) R \frac{\partial H}{\partial R} + \frac{1 - H}{1 + (M - 1) H} \right]_{R=0} = 1. \quad (2.51)
\]

Thus, we have obtained the appropriate boundary and initial conditions for the numerical study, i.e., Equation (2.48), (2.49) and (2.51). A central-difference scheme is employed to provide the numerical solutions (Kurganov and Tadmor, 2000).
2.B Appendix: Derivation of boundary condition (2.16b)

We first note that Equation (2.15) can be rearranged as

\[
\eta - 2M + \frac{4\Gamma M (1 - H) \partial H}{1 + (M - 1)H} \frac{dH}{d\eta} + \frac{4\Gamma MH (1 - H)}{1 + (M - 1)H} = 0. \tag{2.52}
\]

Using boundary condition (2.16a), i.e., \(H(\eta_{N1}) = 0\), we evaluate each term in Equation (2.52) as \(\eta \to \eta_{N1}\). We further assume \(\lim_{\eta \to \eta_{N1}} H \frac{dH}{d\eta} = 0\) and \(\lim_{\eta \to \eta_{N1}} H \frac{d^2H}{d\eta^2} = 0\), and obtain

\[
\left. \left( \eta - 2M + 4\Gamma M \eta \frac{dH}{d\eta} \right) \frac{dH}{d\eta} \right|_{\eta \to \eta_{N1}} = 0. \tag{2.53}
\]

Then, we obtain two values for the slope of the interface \(dH/d\eta\) as \(\eta \to \eta_{N1}\):

\[
\left. \frac{dH}{d\eta} \right|_{\eta \to \eta_{N1}} = 0, \quad \text{and} \quad \left. \frac{dH}{d\eta} \right|_{\eta \to \eta_{N1}^+} = \frac{1}{2\eta_{N1} \Gamma} - \frac{1}{4\Gamma M}. \tag{2.54a,b}
\]

The nontrivial slope (2.54b) is used in the shooting procedure, together with the other boundary condition (2.16a), to solve Equation (2.15).

2.C Appendix: Negligible influence of the slow front

When solving for the interface shape \(f\) using Equation (2.44) subject to boundary conditions (2.45a,b), we have neglected the influence of the slow front at the bottom boundary. Here we investigate under which conditions this is a good approximation.

From Equation (2.44), we obtain that \(f|_{y \to 0} \to -\infty\); thus, the interface \(f\) always intersects with the bottom boundary where \(H = 1\), or equivalently, \(f = \Gamma M/\eta_{N1}\). We now define \(y_{N2}\) as

\[
y_{N2} \equiv \eta_{N2}/\eta_{N1}, \tag{2.55}
\]
Figure 2.10: The location of the slow front $y_{N2}$, defined in (2.55), and the error for the global mass $E_m$, defined in (2.56), both appear to decay exponentially versus $M\Gamma$ from our numerical simulation. In addition, when $M\Gamma \gg 1$, both $y_{N2}$ and $E_m$ are negligibly small for the analysis in Section 2.5 (Regime IV).

which represents the location of the slow front. In addition, we define the error for the global mass $E_m$ introduced by not considering the slow front $y_{N2}$ as

$$E_m \equiv \left| \frac{y_{N2}}{\eta_{N1}} + \int_{y_{N2}}^{1} f \, dy - \int_{0}^{1} f \, dy \right| / \int_{0}^{1} f \, dy. \quad (2.56)$$

Both the location of the slow front $y_{N2}$ and the error $E_m$ are functions of $M\Gamma$, which can be computed from the numerical solution to Equation (2.44) subject to boundary conditions (2.45a,b), as shown in Figure 2.10. From numerical simulation, both $y_{N2}$ and $E_m$ appear to decay exponentially versus $M\Gamma$, and this is consistent with the asymptotic behavior as $y \to 0^+$, see Equation (2.16a) in Lyle et al. (2005). In particular, when $M\Gamma \approx 5$, we obtain $y_{N2} \approx 10^{-3}$, and $E_m \approx 10^{-2}$. We note that in Regime IV, $M\Gamma \gg 1$ always holds; thus, the influence of the slow front $y_{N2}$ is negligibly small in computing the location of the fast front $y_{N1}$ and the shape of the fluid-fluid interface away from the narrow region near the injection site.
Chapter 3

Flow Regime Analysis for Geologic CO$_2$ Sequestration and Other Subsurface Fluid Injections

This chapter uses the flow regime diagram developed from Chapter 2 by analyzing the data collected from the literature, to identify the kinds of analytical solutions appropriate for a range of practical subsurface fluid injection applications. This chapter is adopted from:


3.1 Abstract

Carbon dioxide (CO$_2$) injection into a confined saline aquifer may be modeled as an axisymmetric two-phase flow problem. Assuming CO$_2$ and brine segregate quickly in the vertical direction due to strong buoyancy, and neglecting capillary pressure and miscibility, the lubrication approximation leads to a one-dimensional nonlinear advection-diffusion
equation that describes the evolution of the sharp CO$_2$-brine interface. The interface evolution is driven by two forces: the force from fluid injection, and buoyancy. Analytical solutions can be derived when one of the two forces is dominant. Those solutions depend on the viscosity ratio ($M$) between the displaced and injected fluids, and a buoyancy parameter ($\Gamma$) that measures the relative importance of buoyancy and the driving force from injection. Different combinations of these two parameters give different forms of the solutions. But for all the solutions, the radius of the lateral spreading of the injected fluid follows $r \propto t^{1/2}$, with the proportionality coefficient differing for the different solutions.

In this chapter, we identify the kinds of solutions appropriate for practical CO$_2$ injection projects as well as other subsurface fluid injection applications. We use data from eight CO$_2$ injection projects, 24 acid gas injection projects, two liquid waste disposal projects, and one CO$_2$-WAG enhanced oil recovery project. The solutions provide a simple guidance tool for expected behavior of the different injection operations while providing general insights into overall fluid behavior.

### 3.2 Introduction

Sequestration of carbon dioxide (CO$_2$) into deep saline aquifers is considered a promising technology to mitigate anthropogenic CO$_2$ emissions into the atmosphere (Pacala and Socolow, 2004; IPCC, 2005; Michael et al., 2010). CO$_2$ injection into a saline aquifer involves flow of both the injected CO$_2$ and the resident brine. Understanding such multiphase flows is important to address questions related to CO$_2$ injectivity containment of both CO$_2$ and brine, and the overall long-term effectiveness of the storage operation.

Injection depths are usually chosen so that the injected CO$_2$ will be in a supercritical state. While the supercritical CO$_2$ has density much larger than gaseous CO$_2$, it is still small relative to the density of the resident brine, with a difference ranging from 250 kg/m$^3$ to up to 950 kg/m$^3$, depending on formation depth, geothermal gradient, pressure gradient,
surface temperature, and water salinity (Nordbotten and Celia, 2012). Such density differences lead to strong buoyancy that drives CO$_2$ upward, which leads to vertical segregation between CO$_2$ and brine in the geologic formation. When the time scale associated with buoyant segregation is small relative to the time scales for horizontal propagation, we can assume that the buoyant segregation has occurred, and that CO$_2$ and brine have reached equilibrium in the vertical direction. This vertical equilibrium assumption has been considered to be reasonable, especially at later times in the injection process (Lyle et al., 2005; Nordbotten and Celia, 2006; Nilsen et al., 2011; Court et al., 2012; Pegler et al., 2014; Zheng et al., 2015a) as well as the subsequent post-injection time period (Hesse et al., 2008; Gasda et al., 2011; Szulczewski et al., 2012). Further assumptions of negligible capillary pressure and negligible miscibility between CO$_2$ and brine lead to a model where the less-dense injected fluid overrides the displaced (more dense) fluid and the two fluids form a sharp fluid-fluid interface (see Figure 3.1). Throughout this chapter, we will con-
sider a general set of injected and displaced fluids, not necessarily CO$_2$ and brine, since the methodology also applies to other subsurface fluid injection processes such as acid gas injection and liquid waste disposal.

We assume a homogeneous geologic formation with simple geometries, e.g., horizontal caprock and bedrock. For the vertical equilibrium and sharp interface model, we can derive a one-dimensional (1D) nonlinear advection-diffusion equation for the propagation of the CO$_2$-brine sharp interface. Here, we focus on injection through vertical wells, which corresponds to an axisymmetric flow and for which similarity solutions can be found ([Lyle et al., 2005; Nordbotten and Celia, 2006; Guo et al., 2016]). In the vertical equilibrium model, the vertical flow is negligible as the two fluids are assumed to have already segregated. The horizontal flow is driven by two forces: the force from the fluid injection process, and buoyancy. Analytical solutions can be derived when one of the two forces is dominant. Recently, for this injection scenario and assumptions, [Guo et al., 2016] developed a flow regime diagram to identify the range of applicability of the different solutions to this problem, with the axes of the diagram being the viscosity ratio $M$ between the displaced and the injected fluid and a buoyancy parameter $\Gamma$ that measures the relative importance of buoyancy and the force from injection. The diagram has five flow regimes, four of which have analytical solutions (see Figure 3.2). Regimes I – III are for injection-dominated (injection-driven) flow, but with the injected fluid being more viscous, equally viscous, and less viscous than the displaced fluid, respectively. Regime IV corresponds to buoyancy-dominated (buoyancy-driven) flow, where the flow behavior does not depend on the viscosity ratio. And Regime V is a transition regime, in which the forces from fluid injection and buoyancy are comparable, and where no analytical solution is available. The radius of the lateral fluid spreading follows $r \propto t^{1/2}$ in all flow regimes, while the lateral area of spreading ($\pi r_N^2(t)$) normalized by that of a piston-like spreading is time-independent and is different for each solution (see Figure 3.2).
The purpose of this chapter is to analyze various injection scenarios and place them in the context of this regime diagram. We use data from eight CO$_2$ sequestration projects, 24 acid gas injection operations, two waste disposal projects, and one CO$_2$-WAG enhanced oil recovery project. Each of these projects is characterized by the associated dimensionless groups $M$ and $\Gamma$, thereby placing each project into one of the flow regimes. For the CO$_2$ injections, when the project is a pilot-scale study, we also consider how the characterization would change were the injection to be scaled up to an industrial rate.

### 3.3 The flow regime diagram

In this section, we briefly review the flow regime diagram from [Guo et al.](2016), and highlight some of the flow features in the model of injection and fluid spreading. We consider a horizontal geologic formation with a thickness of $h_0$ (Figure 3.1). The formation is characterized by its porosity and permeability, denoted by $\phi$ and $k$ respectively; $\Delta \rho = \rho_d - \rho_i$ is the density difference between the displaced ($\rho_d$) and the injected ($\rho_i$) fluids and the fluids are assumed incompressible; $\mu_i$ and $\mu_d$ are viscosities of the injected and the displaced fluids, respectively; and $q$ is the volumetric injection rate. It is natural to use cylindrical coordinates and assume an axisymmetric solution. We consider the vertical equilibrium and sharp interface model, and define $h(r,t)$ as the (saturated) thickness of the injected fluid as a function of the radial distance from the injection well and time $t$. $r_{N_1}(t)$ is defined as the leading edge of the plume of the injected fluid (Figure 3.1). For this flow system, we can define two dimensionless groups to characterize the flow behaviors,

$$M \equiv \frac{\mu_d}{\mu_i}, \quad \Gamma \equiv \frac{2\pi \Delta \rho gkh_0^2}{\mu_d q} \quad (3.1)$$

By definition, $M$ is the viscosity ratio between the displaced and the injected fluids, and $\Gamma$ is a buoyancy parameter, which represents the relative importance of buoyancy and the force from fluid injection. The two dimensionless groups $M$ and $\Gamma$ serve to organize the
injection process as they combine fluid properties, geological parameters and the injection rate. A brief derivation of the governing equations is provided for the vertical equilibrium and sharp interface model in Appendix 3.A. The various associated model assumptions are addressed in Appendix 3.B.

For the vertical equilibrium and sharp interface model, four analytical solutions can be derived in four distinct asymptotic limits (flow regimes) with respect to \( M \) and \( \Gamma \). We summarize the solutions for the four flow regimes (Regimes I – IV) in Table 3.1. The solutions are derived with dimensionless variables, which are rescaled as \( H = h/h_0, R = r/h_0, \) and \( T = t/(2\pi\phi h_0^3/q) \). Regimes I – III are for injection-driven flow (\( \Gamma \ll 1 \)), with the injected fluid being more viscous, equally viscous, and less viscous than the displaced fluid for Regimes I, II, and III, respectively. Regime IV has buoyancy-driven flow (\( \Gamma \gg 1 \)), where the flow behavior does not depend on the viscosity ratio. By comparing the analytical solutions with the full numerical solution, we can obtain a flow regime diagram that organizes the kind of flow behaviors that are expected (Guo et al., 2016) (see Figure 3.2). The boundaries between the flow regimes are defined as the values that introduce only a 10% difference when the respective analytical solution is compared to the full numerical solution, with the difference measured using the similarity transformed (\( \eta_{N_i} = R_{N_i}^2/T \)) location of the leading edge of the CO\(_2\) plume. The location of the leading edge of the CO\(_2\) plume is chosen because it is an important factor for risk assessment of CO\(_2\) injection, especially for leakage risk assessment. Other criteria may be used to measure the discrepancy, such as the difference associated with the approximate shape of the entire fluid-fluid interface, or the difference in the trailing edge. Different criteria may give quantitatively different regime boundaries, but they will not qualitatively change the flow regime diagram.

We can use this regime diagram to study a practical injection project by computing the dimensionless groups \( M \) and \( \Gamma \) from Equation (3.1). Figure 3.2 shows a flow chart that demonstrates a step-by-step procedure for using the flow regime diagram for assessing a practical project. Different flow regimes have different engineering implications, e.g.,
Regimes | \((M, \Gamma)\) | Interface shape | Leading edge | Trailing edge |
---|---|---|---|---|
I | \(M < 1, \Gamma \ll 1\) | \(H(R, T) = \frac{M-1}{4M} \left(\frac{R^2}{T} - 2\right) + 1/2\) | \((2 + \frac{2\Gamma}{1-M})^{1/2} T\) | \((2 - \frac{2\Gamma}{1-M})^{1/2} T\) |
II | \(M = 1, \Gamma \ll 1\) | \(H(R, T) = \frac{R^2}{4\sqrt{T}} + 1/2\) | \((2 + 2\sqrt{T})^{1/2} T\) | \((2 - 2\sqrt{T})^{1/2} T\) |
III | \(M > 1, \Gamma \ll 1\) | \(H(R, T) = \left(\sqrt{2M/(R^2/T)} - 1\right)/(M-1)\) | \((2M)^{1/2} T\) | \((2/M)^{1/2} T\) |
IV | any \(M, \Gamma \ll 1\) | Obtain by numerical integration | \((11.2\Gamma M)^{1/4}\) | No trailing edge |

Table 3.1: A summary of the analytical solutions for flow Regimes I - IV for nearly horizontal flows in a confined reservoir. The solutions are written in terms of the dimensionless variables. As shown in Figure 3.1, we define the intersections between the interface and the top and bottom boundaries of the aquifer as edges of the plume of the injected fluid. The leading edge measures the furthest distance the CO$_2$ travels from the injection well at any given time. The trailing edge denotes the intersection of the interface with the bottom boundary; there is no trailing edge when the interface does not intersect the bottom boundary. \(M\) and \(\Gamma\) are defined in Equation (3.1).

Different regimes have different area of spreading for a given amount of injected fluid. To understand the area of spreading we introduce the concept of normalized area of impact, which is defined as the lateral radial area occupied by a given volume of injected fluid normalized by the lateral radial area from a piston-like displacement (where the fluid-fluid interface is vertical). The greater is the normalized area, the further a given amount of the injected fluid spreads. The analytical expressions for the normalized area of impact for each of the regimes are presented in Figure 3.2, where we also show an example calculation to give a sense of the values of the normalized areas of impact, which are independent of time. The results show that the buoyancy-driven regime has a much larger area of impact compared to the injection-driven regimes for a fixed volume of injected fluid, and for the injection-driven solutions, higher viscosity ratios lead to more spreading. The transition regime would have an area of impact in between the injection-driven and buoyancy-driven flow regimes.
Figure 3.2: A flow chart demonstrating the procedure for using the flow regime diagram from [Guo et al., 2016] to investigate a practical project. For a specific project, a pair of \((M, \Gamma)\) values can be computed from the reported parameters. When the pair of \((M, \Gamma)\) is in Regimes I - IV, the fluid propagation has an analytical solution, otherwise it enters Regime V, where no analytical solution is available. The sketches corresponding to each of the flow regimes show the fluid-fluid interface shapes for different analytical solutions. For each case, the time dependence of the spreading of the injected fluid can be evaluated. We also show the expressions of the normalized area of impact, which is time-independent, for all the solutions. An example calculation is shown with the values for and for the four regimes as: (I) \(M = 0.1, \Gamma = 8.5\); (II) \(M = 1, \Gamma = 0.1\); (III) \(M = 10, \Gamma = 0.9\); (IV) \(M = 10, \Gamma = 36\).
3.4 Flow regime analysis

In this section, we use the flow regime diagram to study various kinds of injection operations. Detailed data for different projects are given in Tables 3.2 and 3.3. Further information about the data and the calculations is provided in Appendix 3.C and 3.D.

3.4.1 Geologic CO₂ sequestration

The values of dimensionless groups \( (M, \Gamma) \) for eight CO₂ injection projects are shown in Figure 3.3 with an associated range of variations in \( \Gamma \). The percentages indicate the difference between the analytical solution of Regime III and the full solution. The range of \( \Gamma \) values is based on identified ranges of parameters, with most of the variation being associated with values of the permeability. Variations in \( M \) are small, and are therefore not shown. Detailed data and estimates of the variations are given in Table 3.2 and Appendix 3.C. Since the injected CO₂ is always less viscous than the resident brine in the aquifers \( (M > 1) \), all the projects fall on the right side of the regime diagram (Figure 3.3). The injection-driven regime (Regime III) has three projects, corresponding to the Sleipner 9th layer, In Salah, Decatur, and Snøhvit. The transition regime (Regime V) includes the other five projects: Ketzin, Frio, Cranfield, Decatur, and Gorgon.

The three projects in the injection-driven regime (Regime III) all have relatively large injection rates, with a single-well injection rate of CO₂ larger than 0.3 Mt/year. We note that a larger injection rate leads to a smaller \( \Gamma \), see Equation (3.1). Physically this means that the flow is mainly driven by fluid injection instead of buoyancy. The total injection rate in In Salah was reported to be about 1.28 Mt/year \( (Michael et al., 2010) \), and CO₂ was injected through three horizontal wells. We only consider the injection well KB-501, which has an average injection rate of around 0.3 Mt/year. Since we only look at the long-term behavior of the CO₂ plume, we treat the injection well as a point source equivalent to a vertical well. For the Sleipner project, we only consider CO₂ migration in the upper-most
(the 9th) layer and treat the input source of CO$_2$ from below as a continuous injection. The mass rate of CO$_2$ “injection” into the upper-most layer is reported to have increased from 0.02 Mt/year in 1999 to 1.56 Mt/year in 2009 (Singh et al., 2010). Here we consider the CO$_2$ flow behavior from 2005 to 2009 when the mass rate was between around 0.5 Mt/year and 1.56 Mt/year, and use an average mass rate of 1 Mt/year to do the analysis. We note that the CO$_2$ flow will likely be in the buoyancy-driven regime (Regime IV) in the early years when the CO$_2$ “injection” rate was small. For the Snøhvit project, it has been shown that CO$_2$ was contained in Tubåen 1 by the overlying shale unit (Grude et al., 2014); thus, we only consider the Tubåen 1 sandstone unit in the lower part of the Tubåen formation.

The three pilot projects (Keztin, Frio, and Cranfield) and the Gorgon and Decatur projects are all in the transition regime (Regime V). Among the three pilot projects, Cranfield has the largest injection rate (0.14 Mt/year). The Gorgon project has an injection rate of 0.56 Mt/year for a single well, but it is still in the transition regime due to its reported large thickness $h_0 = 250$ m, which leads to a large value of $\Gamma$. The Decatur project is near the boundary of Regimes III and V, being slightly in Regime V.

We next consider scenarios where all the projects are scaled up to an industrial scale, with injection rates increased to 1 Mt/year, because any actual practical project would necessarily inject large amounts of CO$_2$ (IPCC, 2005; Michael et al., 2010). With the increased injection rate, all of the $(M, \Gamma)$ pairs for the pilot projects shift down to the injection regime as shown in Figure 3.4, with only the Gorgon project remaining in Regime V (due to its very large formation thickness). These calculations suggest that the analytical solution of Regime III is the appropriate choice for the sharp-interface model involving large-scale CO$_2$ injection.

### 3.4.2 Other subsurface fluid injection projects

We have also computed the dimensionless pairs $(M, \Gamma)$ for 24 acid gas injection projects, based on data from Bachu et al. (2005), and placed them onto the flow regime diagram.
Figure 3.3: Flow regime diagram for eight CO$_2$ injection projects in saline aquifers. The open markers represent projects with industrial-scale injection rates, and the closed markers filled by blue color indicate the projects with pilot-scale injection rates. The five flow Regimes I - V are separated by black dash-dot lines (Guo et al., 2016). The numbers marked besides each point are the differences introduced at the location of the leading edge if the analytical solution of Regime III is used instead of the numerical solution to the corresponding boundary value problem. Detailed data for computing $M$ and $\Gamma$ can be found in Table 3.2 and in Appendix 3.C.

(see Figure 3.5). The majority of the projects (16 out of 24) go into the injection-driven regime (Regime III), one project lies in the buoyancy-driven regime (Regime IV), and seven projects lie in the transition regime (Regime V). We note that $\Gamma$ is small for many of the acid gas projects although the injection rates are not large, which is mainly because the formations are reported to be thin and have low permeability. Detailed data for the acid gas injection projects is provided in Appendix 3.D.

In addition, we considered a CO$_2$-WAG EOR project and two subsurface waste disposal projects. For the CO$_2$-WAG EOR project, we focus on the fluid-fluid interface between water and CO$_2$, which includes (more viscous) water pushing (less viscous) CO$_2$, as well
Figure 3.4: Flow regimes for the eight CO₂ injection projects into saline aquifers with a (hypothetical) industrial-scale injection rate of 1 Mt/year.

<table>
<thead>
<tr>
<th>Project</th>
<th>Scale</th>
<th>( h_0 ) (m)</th>
<th>( \phi ) (-)</th>
<th>( k ) (mD)</th>
<th>( q ) (Mt/y)</th>
<th>( M ) (-)</th>
<th>( \Gamma ) (-)</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ketzin</td>
<td>Pilot</td>
<td>73</td>
<td>0.23</td>
<td>100</td>
<td>0.01</td>
<td>19.08</td>
<td>16.90</td>
<td>49.3</td>
</tr>
<tr>
<td>Cranfield</td>
<td>Pilot</td>
<td>24</td>
<td>0.30</td>
<td>270</td>
<td>0.14</td>
<td>5.23</td>
<td>1.42</td>
<td>27.2</td>
</tr>
<tr>
<td>Frio</td>
<td>Pilot</td>
<td>24</td>
<td>0.30</td>
<td>1400</td>
<td>0.09</td>
<td>12.34</td>
<td>5.45</td>
<td>35.7</td>
</tr>
<tr>
<td>Decatur</td>
<td>Demonstration</td>
<td>46</td>
<td>0.15</td>
<td>120</td>
<td>0.37</td>
<td>6.28</td>
<td>0.25</td>
<td>11.3</td>
</tr>
<tr>
<td>Sleipner</td>
<td>Commercial</td>
<td>11.3</td>
<td>0.36</td>
<td>2000</td>
<td>1</td>
<td>13.33</td>
<td>0.12</td>
<td>1.4</td>
</tr>
<tr>
<td>Snøhvit</td>
<td>Commercial</td>
<td>14</td>
<td>0.19</td>
<td>750</td>
<td>0.30</td>
<td>8.07</td>
<td>0.60</td>
<td>8.9</td>
</tr>
<tr>
<td>In Salah</td>
<td>Commercial</td>
<td>20</td>
<td>0.17</td>
<td>20</td>
<td>0.30</td>
<td>5.77</td>
<td>0.03</td>
<td>2.1</td>
</tr>
<tr>
<td>Gorgon</td>
<td>Commercial</td>
<td>250</td>
<td>0.20</td>
<td>25</td>
<td>0.56</td>
<td>7.02</td>
<td>4.36</td>
<td>42.8</td>
</tr>
</tbody>
</table>

Table 3.2: Data and parameters for CO₂ sequestration projects in saline aquifers. \( h_0 \) is the thickness of the aquifer, \( \phi \) is porosity, \( k \) is porosity, \( q \) is the mass injection rate for a single well, and \( M \) and \( \Gamma \) are the dimensionless groups defined in Equation (3.1).
Table 3.3: Parameters and data for CO₂-WAG EOR and waste disposal project. \( \rho_d \) and \( \rho_i \) are density of the displaced fluid and the injected fluid, respectively; \( \mu_d \) and \( \mu_i \) are the viscosity of the displaced fluid and the injection fluid, respectively. Other variables have the same definitions as those in Table 3.2.

<table>
<thead>
<tr>
<th>Project</th>
<th>( h_0 ) (m)</th>
<th>( \phi ) (-)</th>
<th>( k ) (mD)</th>
<th>( \rho_d ) (kg/m³)</th>
<th>( \mu_d ) (m Pa s)</th>
<th>( \rho_i ) (kg/m³)</th>
<th>( \mu_i ) (m Pa s)</th>
<th>( q ) m³/s</th>
<th>( M ) (-)</th>
<th>( \Gamma ) (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waste disposal 1</td>
<td>15.2</td>
<td>0.07</td>
<td>69</td>
<td>1094</td>
<td>0.893</td>
<td>1006</td>
<td>0.668</td>
<td>0.0063</td>
<td>1.35</td>
<td>0.02</td>
</tr>
<tr>
<td>Waste disposal 2</td>
<td>50</td>
<td>0.32</td>
<td>695</td>
<td>1085</td>
<td>0.686</td>
<td>1195</td>
<td>1.220</td>
<td>0.0033</td>
<td>0.56</td>
<td>5.28</td>
</tr>
<tr>
<td>EOR (water to CO₂)</td>
<td>81</td>
<td>0.04</td>
<td>19.4</td>
<td>670</td>
<td>0.062</td>
<td>994</td>
<td>0.445</td>
<td>0.16</td>
<td>0.14</td>
<td>0.26</td>
</tr>
<tr>
<td>EOR (CO₂ to water)</td>
<td>81</td>
<td>0.04</td>
<td>19.4</td>
<td>994</td>
<td>0.445</td>
<td>670</td>
<td>0.062</td>
<td>0.16</td>
<td>7.18</td>
<td>0.04</td>
</tr>
</tbody>
</table>

as CO₂ displacing water. We note that the case of water pushing CO₂ has a more dense fluid displacing a less dense fluid, where the fluid-fluid interface should be flipped upside down compared to that of a less dense fluid displacing a more dense fluid (see Figure 3.1).

Based on the parameters from Kane (1979), these two displacement cases fall in Regimes I and III. The two waste disposal projects include liquid waste injection into a carbonate aquifer and a sandstone aquifer, respectively. Depending on the salinity of the injected and displaced fluids, for a waste disposal project, the injected fluid can be either more viscous or less viscous than the displaced fluid. Here we use the parameters from Ortoleva and Liu (1995) and consider two scenarios. One corresponds to the buoyancy-driven regime (Regime IV) and the other lies in the injection-driven regime (Regime III), as shown in Figure 3.5.

### 3.5 Conclusions

In this chapter, we collected data from various injection projects that involve fluid injection into deep formations and investigated the flow behaviors for each of the projects, using the flow regime diagram from Guo et al. (2016). Among the eight geologic CO₂ sequestration projects we considered, including both industrial-scale and pilot-scale projects, four (all industrial-scale) fall within in the injection-driven regime (Regime III), while the other
Figure 3.5: Flow regime diagram for eight CO₂ injection projects, 24 acid gas injection projects, two waste disposal projects, and one CO₂-WAG EOR project.

Four (mostly pilot-scale) are in the transition regime (Regime V). We note that although the regime of a project depends on various parameters that contribute to the dimensionless groups \((M, \Gamma)\), the injection rate is a significant controlling parameter. If an industrial-scale injection rate of 1 Mt/year is applied to the pilot-scale projects, all three projects move into the injection-driven regime (Regime III). In addition to CO₂ injection, we showed that almost all of the acid-gas injection operations fall within Regime III or V, while CO₂-WAG EOR and liquid waste disposal injections can populate Regimes I, II, and IV. This flow regime analysis provides insights into the flow processes and serves to guide the choice of simplified models and analytical solutions that can be applied to different kinds of injection scenarios. Finally, we have noted that the normalized area of spreading is time independent and only depends on the associated values of \(M\) and \(\Gamma\).
3.A Appendix: The model

In this section, we give a brief summary of the vertical equilibrium and sharp interface model from [Guo et al. (2016)]. As shown in Figure 3.1, we consider a horizontal geologic formation with a thickness \( h_0 \); \( \phi \) and \( k \) are the porosity and permeability of the geologic formation, respectively; \( \Delta \rho = \rho_d - \rho_i \) is the density difference between the displaced (\( \rho_d \)) and the injected (\( \rho_i \)) fluids; \( \mu_i \) and \( \mu_d \) are viscosities of the injected and the displaced fluids, respectively; and \( q \) is the volumetric injection rate. It is natural to use cylindrical coordinates and assume an axisymmetric solution, and we define \( h(r,t) \) as the (saturated) thickness of the injected fluid as a function of the radial distance \( r \) from the injection well and time \( t \). \( r_{N_1}(t) \) is defined as the leading edge of the plume of the injected fluid.

By combining the mass balance equations and the volumetric flux equation (Darcys equation), we obtain a 1D nonlinear advection-diffusion equation for the propagation of the fluid-fluid interface \( h(r,t) \)

\[
\frac{\partial h}{\partial t} = \frac{1}{\phi r} \frac{\partial}{\partial r} \left( \frac{\Delta \rho g k h (h_0 - h)}{\mu_d h + \mu_i (h_0 - h)} \frac{\partial h}{\partial r} + \frac{q \mu_i (h_0 - h)}{2 \pi (\mu_d h + \mu_i (h_0 - h))} \right). \tag{3.2}
\]

We consider a geologic formation whose pore space is originally filled with the displaced fluid, thus the initial condition is

\[
h(r,0) = 0. \tag{3.3}
\]

Two boundary conditions are needed. One is at the leading edge \( (r_{N_1}(t)) \) of the plume of the injected fluid, where the height of the injected fluid is zero; the other is at the origin (the location of the injection well), where the volumetric injection rate is \( q \). The conditions are

\[
h(r_{N_1}(t)) = 0, \tag{3.4}
\]

\[
\left[ \frac{\Delta \rho g k h (h_0 - h)}{\mu_d h + \mu_i (h_0 - h)} \frac{\partial h}{\partial r} + \frac{q \mu_i (h_0 - h)}{2 \pi (\mu_d h + \mu_i (h_0 - h))} \right] \bigg|_{r=0} = 0. \tag{3.5}
\]
where Equation (3.5) is obtained by integrating Equation (3.2) with respect to $r$ from the origin to the leading edge of the plume.

A non-dimensional version of Equation (3.2) can be obtained by defining $H = h/h_0$, $R = r/h_0$, $T = t/((2\pi\phi h_0^2)/q)$, and using these to transform to an equation for $H(R, T)$:

$$
\frac{\partial H}{\partial T} = \frac{1}{R} \frac{\partial}{\partial R} \left( \frac{\Gamma MH(1 - H)R \partial H}{1 + (M - 1)H} \right),
$$

(3.6)

where we define two dimensionless groups

$$
M \equiv \frac{\mu_d}{\mu_i} \quad \text{and} \quad \Gamma \equiv \frac{2\pi\Delta \rho gkh_0^2}{\mu_d q}.
$$

(3.7a, b)

By definition, $M$ is the viscosity ratio between the displaced fluid and the injected fluid, and $\Gamma$ is a buoyancy parameter, which represents the relative importance of buoyancy and the force from fluid injection.

The dimensionless form of the initial and boundary conditions can also be derived. Then, with the definition of the similarity variable $\eta = R^2/T$, Equation (3.6) becomes an ordinary differential equation

$$
\eta \frac{dH}{d\eta} + 2 \frac{d}{d\eta} \left( \frac{2\Gamma MH(1 - H)\eta}{1 + (M - 1)H} \frac{dH}{d\eta} + \frac{1 - H}{1 + (M - 1)H} \right) = 0.
$$

(3.8)

The two boundary conditions with respect to the new variable $\eta$ can also be derived. Equation (3.8), in general, does not have analytical solutions, but it can be solved analytically in the four asymptotic limits. The four analytical solutions are summarized in Table 3.1 which correspond to Regimes I, II, III, and IV. We note that the form of the similarity variable implies that the location of the leading edge follows $R_{N_i} \propto T^{1/2}$. Thus, relative to a uniform injection front, i.e. piston-like injection, which also would advance proportional to $T^{1/2}$, the ratio of the lateral area of spreading for a given volume of injected fluid between the analytical solutions and piston-like injection is independent of time.
3.B Appendix: Model assumptions

In this section, we discuss the assumptions and limitations for the vertical equilibrium and sharp interface model.

The entire analysis of this chapter relies on the vertical equilibrium and sharp interface assumptions. The validity of the vertical equilibrium assumption depends on the time scale associated with the vertical buoyant segregation and the aspect ratio (length to thickness) of the aquifer. Lake (1989) and Yortsos (1995) discussed the appropriateness of the vertical equilibrium assumption with respect to the aspect ratio of the geometry of the geologic formation and the difference between the permeabilities in the horizontal and vertical directions. Nordbotten and Dahle (2011) analyzed the impact of the capillary transition zone on the vertical equilibrium models and Court et al. (2012) investigated the validity of the vertical equilibrium and sharp interface assumptions in practical simulations for CO₂ storage.

The vertical equilibrium assumption has been generally considered reasonable for homogeneous geologic formations with relatively high permeability. This is especially true for later times during the injection period and the subsequent post-injection time period. For geologic formations with low permeability and heterogeneities, the time scale for the assumption to be valid may be longer, and other solution strategies need to be applied (see Chapter 4).

Here, we estimate the time scale of vertical segregation and the travel distance of the injected fluid plume for which the vertical equilibrium assumption is applicable. The time scale for the two fluids to segregate \( t_s \) in the vertical direction can be estimated as

\[
t_s \approx \frac{h_0 \phi}{\Delta \rho g k_z \lambda_d^*},
\]

where \( k_z \) is the vertical permeability of the geologic formation, and \( \lambda_d^* = k_{r,d}^*/\mu_d \) indicates the characteristic mobility of the displaced fluid, with \( k_{r,d}^* \) being the characteristic relative permeability for the displaced fluid. For the vertical equilibrium assumption to be valid,
the time of horizontal spreading \((t)\) needs to be larger than the segregation time scale \((t_s)\), i.e
\[
t \geq t_s.
\] (3.10)

Now, we estimate the horizontal distance the injected fluid travels for time \(t\). Here, we consider an example of a less viscous fluid displacing a more viscous fluid in both the buoyancy-driven and the injection-driven cases.

For the buoyancy-driven regime, the leading edge of the injected fluid follows
\[
\frac{R_{N_1}^2}{T} = \left(\frac{2\Gamma M}{0.18}\right)^{1/2},
\] (3.11)

Thus,
\[
t = T \frac{2\pi \phi h_0^3}{q} = R_{N_1}^2 \left(\frac{0.18}{2\Gamma M}\right)^{1/2} 2\pi \phi h_0^3 \frac{q}{Q}.
\] (3.12)

Substituting \(t \geq t_s\) to Equations (A8) and (A11), we obtain
\[
R_{N_1} \geq (k_x/k_z)^{1/2}(M/\Gamma)^{1/4}(1/k_{r,d}^*)^{1/2}(2/0.18)^{1/4}.
\] (3.13)

We choose a typical value of \((M,\Gamma) = (8,32)\) in the buoyancy-driven regime, the representative relative permeability \(k_{r,d}^* = 1\), and use a horizontal-to-vertical anisotropy ratio of permeabilities \(k_x/k_z = 10\). Then, we get \(R_{N_1} \geq 4\), which suggests that the horizontal distance of the injected fluid \(r_{N_1} = R_{N_1} h_0\) needs to be larger than 4 times the thickness of the geologic formation, that is \(r_{N_1} \geq 4h_0\), for the vertical equilibrium assumption to be valid in the buoyancy-driven regime. We note that this estimate depends on \(k_{r,d}^*\), which can vary between 0 and 1. For example, \(R_{N_1} \geq 13\) for \(k_{r,d}^* = 0.1\). For the injection-driven regime, the leading edge of the injected fluid follows
\[
\frac{R_{N_1}^2}{T} = 2M.
\] (3.14)
Similarly, we can obtain

\[ R_{N_1} \geq (k_x/k_z)^{1/2}(2M/\Gamma)^{1/2}(1/k_{r,d}^*)^{1/2}. \]  \hspace{1cm} (3.15)

A typical value of \((M,\Gamma) = (8,0.1), k_{r,d}^* = 1,\) and \(k_x/k_z = 10\) provide \(R_{N_1} \geq 40.\) Thus, the horizontal distance of the injected fluid needs to be larger than 40 times the thickness of the geologic formation. We also note that \(R_{N_1} \geq 125\) for \(k_{r,d}^* = 0.1.\)

When the driving forces from buoyancy and fluid injection are comparable, the horizontal traveling distance is expected to be in between of the estimates for the buoyancy-driven and the injection-driven flow regimes.

### 3.C Appendix: Data for CO\(_2\) injections

Here we show date collected from the literature and computed values of \(M\) and \(\Gamma\) for the 8 CO\(_2\) injection projects (see Table [3.4]).

### 3.D Appendix: Data for acid gas injections

In this Appendix, we provide the data collected from the literature and computed values of \(M\) and \(\Gamma\) for the 24 acid injection projects (see Table [3.5]).
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Table 3.4: $\rho_b$ and $\rho_c$ are brine and CO$_2$ densities respectively, $\mu_b$ and $\mu_c$ are brine and CO$_2$ viscosities, respectively. For each project, we collect parameters from the literature and compute a reference, an upper bound and a lower bound for the gravity number $\Gamma$. The “-” signs in the data entries indicate that the values are the same as the reference values. The sources of the data are listed in the last column.
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Table 3.5: This table of data is from [Bachu et al., 2005], with corrections made according to the authors.
Chapter 4

A Single-layer Vertically-integrated Model with Vertical Dynamics for CO₂ Sequestration

This chapter is adopted from the publication [Guo et al. (2014a)]:


4.1 Abstract

Conventional vertically-integrated models for CO₂ storage usually adopt a vertical equilibrium (VE) assumption, which states that due to strong buoyancy, CO₂ and brine segregate quickly, so that the fluids can be assumed to have essentially hydrostatic pressure distributions in the vertical direction. However, the VE assumption is inappropriate when the time scale of fluid segregation is not small relative to the simulation time. By casting the vertically integrated equations into a multiscale framework, a new vertically-integrated model
can be developed that relaxes the VE assumption, thereby allowing vertical dynamics to be modeled explicitly. The model maintains much of the computational efficiency of vertical integration while allowing a much wider range of problems to be modeled. Numerical tests of the new model, using injection scenarios with typical parameter sets, show excellent behavior of the new approach for homogeneous geologic formations.

4.2 Introduction

Geological sequestration of carbon dioxide (CO$_2$) has been proposed as a promising mitigation strategy to reduce the global warming effects caused by increasing anthropogenic CO$_2$ emissions (IPCC, 2005). Such technology involves capturing anthropogenic CO$_2$ and injecting the captured CO$_2$ into permeable geologic formations deep in the subsurface. One important type of storage formation is deep saline aquifers, where CO$_2$ would be injected into a formation whose pore space is initially filled with brine. In order to effectively mitigate the global warming problem, geological sequestration of CO$_2$ has to be deployed at a very large scale, with injection increasing to the order of 3.5 billion tons of carbon per year over the next 50 years (Pacala and Socolow, 2004). With such large amounts of fluids being injected, a range of engineering questions have to be answered to determine that the CO$_2$ is safely stored over a long period of time. These questions include the spatial extent of the CO$_2$ plume, the spatial extent of significant pressure perturbations, and the risk of fluid leakage out of the target formation. To answer these questions, mathematical models representing the physical processes of the system are required.

Injection of CO$_2$ into a saline aquifer leads to a flow system with multiple fluid phases, which typically involves an invading less viscous and less dense supercritical CO$_2$ phase and a resident more viscous and denser brine phase. Mathematical models for the multiphase flow system vary across a broad range of complexity, from simplified analytical solutions, (Huppert and Woods, 1995; Lyle et al., 2005; Nordbotten and Celia, 2004).
to full three-dimensional (3D) multiphase multicomponent models, such as ECLIPSE (Geo-Quest, 2010), TOUGH2 (Pruess, 2005), STOMP (White and Oostrom, 1997), and FEHM (Zyvoloski et al., 1997). One family of simplified models has been developed based on the assumption of vertical equilibrium (VE) (Huppert and Woods, 1995; Lyle et al., 2005; Nordbotten and Celia, 2006; Vella and Huppert, 2006; Hesse et al., 2007, 2008; Gasda et al., 2009, 2011; MacMinn et al., 2010). The VE assumption states that brine and CO₂ segregate instantaneously and are therefore at equilibrium in the vertical direction (i.e., the pressure distribution for each fluid is essentially hydrostatic). This assumption implies that the functional form of the phase pressures in the vertical direction is known, a priori. Therefore, the solution in the vertical does not need to be computed, so that the governing equations for the system are integrated across the vertical direction, resulting in a set of equations defined in the horizontal plane. The reduction of spatial dimensions gives significant computational advantages over full three-dimensional models. Such VE models are applicable whenever the VE assumption is satisfied. These kinds of models have been used to study many problems related to geological storage of CO₂ (Bandilla et al., 2012; Court et al., 2012; Gasda et al., 2009, 2011, 2012a; Nilsen et al., 2011; Huang et al., 2014). However, there are a number of cases (see, e.g., Court et al., 2012) for which the VE assumption is inappropriate. For example, for target formations with relatively low vertical permeability, large formation thickness or small density contrast between CO₂ and brine, the two fluid phases may not reach vertical equilibrium for a long period of time. For problems where the VE assumption is not appropriate, vertical dynamics of CO₂ and brine flow should be included in the models. At present, this means use of full three-dimensional models for the multiphase system.

Here we propose a new model that maintains the computational efficiencies of a vertically-integrated model while relaxing the assumption of vertical equilibrium. We cast the new model in a multiscale framework, in direct analogy to the recent presentations.
of VE models (see, e.g. Nordbotten and Celia, 2012). The coarse scale is the horizontal domain, while the fine scale is the vertical domain which corresponds to the thickness of the formation. Because the formation thickness is usually much smaller than the horizontal extent, scale separation is appropriate. As in VE models, a vertically-integrated equation is solved for the pressure defined at the coarse scale. However, in contrast to VE models that solve a second vertically-integrated equation for the vertically-integrated phase saturation, followed by analytical reconstruction of the pressure profiles in the vertical direction, the new algorithm solves locally one-dimensional (vertical) dynamic equations to calculate the vertical transients of the fluid saturation profiles. In these locally one-dimensional equations, fine-scale horizontal fluxes are included as sources and sinks. These fine-scale horizontal fluxes are computed from the reconstructed vertical fine-scale pressure field. The pressure reconstruction is based on the coarse-scale pressure and the vertical structure of the fine-scale pressure field from the previous time step. After computing the vertical (fine-sale) saturation, an updated fine-scale pressure is reconstructed. The end result is an algorithm that maintains the computational efficiency of a vertically-integrated pressure equation while capturing the vertical dynamics of the two-phase flow system.

In this chapter, we provide details and initial computational results for the new algorithm. We first give a brief overview of the basic two-phase flow equations for the CO₂ storage system. This is followed by a review of VE models. We then give a presentation of the new multiscale algorithm that incorporates the vertical dynamics into the vertically-integrated framework. Next, we compare the new multiscale model with a full multi-dimensional model and a VE model to demonstrate its applicability under different conditions. Finally, we summarize the key findings and discuss future extensions and directions.
Figure 4.1: A schematic description of CO$_2$ injection in an aquifer in the $r$ - $z$ cross-section, where a vertical CO$_2$ injection well is placed on the left side ($r = 0$) and a vertical column is highlighted to demonstrate flow dynamics of CO$_2$ and brine. The arrows represent flow directions of the two fluid phases.

4.3 Background

The system of CO$_2$ storage involves a multiphase flow system which requires a set of equations to represent the flow dynamics of each phase. In this section, we will first introduce the basic equations for the multiphase flow system and then review the VE models that approximate the system as two-dimensional by assuming hydrostatic pressure profiles for both phases.

4.3.1 Two-phase flow equations

Injection of CO$_2$ into deep saline aquifers usually leads to a two-phase flow system with the fluids being brine and a CO$_2$-rich phase. Figure 4.1 depicts the flow dynamics of injected CO$_2$ and resident brine, both of which have significant horizontal velocities because of the imposed pressure gradient. In addition, the injected CO$_2$ will move upward driven by buoyancy whereas the resident brine will experience gravity drainage.
The two-phase flow system can be described by a mass conservation equation for each phase. For simplicity, here we do not consider the mutual solubility of the two fluids, that is, the CO$_2$-rich phase only contains CO$_2$ and the brine phase only contains brine. Typically, mass fraction of CO$_2$ component in pure water under typical pressure and temperatures of the geological formation is small (5%), the mass fraction of H$_2$O into pure CO$_2$ phase is even smaller, less than 1% (Nordbotten and Celia, 2012). We note that mutual solubility might be important under certain conditions, e.g. the CO$_2$ dissolution into brine may lead to convective mixing in the vertical direction at large time scales, which may have impact on CO$_2$ migration significantly. However, we chose not to include mutual solubility and CO$_2$ density variations for now, because this chapter only focuses on CO$_2$ injection, the time scale of which is typically short relative to the time scale for convective mixing. The mass balance equation for each fluid phase is given by

$$\frac{∂}{∂t}(ρ_α φ_α s_α) + \nabla \cdot (ρ_α u_α) = ρ_α ψ_α,$$

(4.1)

where $α = b$ or $c$, with $b$ and $c$ representing brine and CO$_2$ respectively, $φ$ is the porosity of the rock, $ρ_α$ is fluid density, $s_α$ is phase saturation, $u_α$ is volumetric flux, and $ψ_α$ is the source or sink term.

The volumetric flux is governed by the two-phase extension of Darcys Law

$$u_α = -\frac{k_{r,α} k}{μ_α} (\nabla p_α - ρ_α g),$$

(4.2)

where $k_{r,α}$ is the relative permeability, assumed here to be scalar function of saturation, $k$ is the intrinsic permeability of the porous medium, $μ_α$ is viscosity, $p_α$ is phase pressure and $g$ is the gravity acceleration vector.

The relative permeability $k_{r,α}$ is usually approximated as an empirical function of phase saturation. The pressure difference between the two phases is defined as the capillary pressure, which is also commonly parameterized as an algebraic function of phase saturation.
That is, we have

\[ k_{r,\alpha} = k_{r,\alpha}(s_{\alpha}), \quad \text{and} \quad p_e - p_b = p_{\text{cap}}. \]

Because the pore space must be occupied by either CO\(_2\) or brine, the saturation of the two fluid phases must sum to unity,

\[ s_b + s_c = 1. \quad (4.4) \]

The above equations form a closed set of equations for the two-phase flow system of CO\(_2\) storage. To study the CO\(_2\) migration and pressure perturbation during and after injection, we need to solve the two-phase flow equations either analytically or numerically.

### 4.3.2 Vertically-integrated approach with static (Dupuit) reconstruction (Vertical Equilibrium)

In this section, we will give a brief overview of VE models. These models assume that the two fluid phases have fully segregated due to buoyancy, and that the phase pressures have reached gravity-capillary equilibrium in the vertical direction. With this assumption, the functional form of the pressure distribution is known, a priori, in the vertical direction. Given the two phase pressures, the capillary pressure function \( p_{\text{cap}}(s_{\alpha}) \) can be inverted to give the associated saturation profile in the vertical. Therefore, no numerical solution is needed in the vertical, and it is natural to integrate the governing equations over the thickness of the formation to derive a two-dimensional equation set. The VE algorithm proceeds with numerical solution of the two-dimensional vertically-integrated equations and an algebraic (analytical) reconstruction of the vertical profiles based on the VE assumption. This provides a solution for the entire three-dimensional system. We refer to this reconstruction in the vertical as a “static” reconstruction, because no dynamics are included in the vertical dimension. We summarize the VE equations in the following.

Figure 4.2 is a schematic diagram of the aquifer system, where \( x_3 \) is the direction orthogonal to the dominant plane of the formation. All “vertical” integrations are performed.
along the $x_3$ direction. Integration of the general three-dimensional Equation (4.1) from the bottom to the top of the aquifer yields

$$\int_{\xi_B}^{\xi_T} \left( \frac{\partial}{\partial t} \left( \rho \alpha u_\alpha \right) \right) dx_3 = \int_{\xi_T}^{\xi_B} \rho_\alpha \psi^\alpha dx_3. \quad (4.5)$$

When the spatial derivative of density can be assumed to be negligibly small, a slight compressibility assumption is introduced for the system: this involves keeping the time derivative terms for density and porosity while neglecting the spatial derivatives of density. This is consistent with many models for subsurface flows (Bear [1972], Gasda et al. [2009], Nordbotten and Celia [2012]). The standard definitions for compressibilities are given below in Equations (4.6) and (4.7).

$$d\rho_\alpha = \frac{d\rho_\alpha}{dp} dp = \rho_\alpha c_\alpha dp \quad (4.6)$$

$$d\phi = \frac{d\phi}{dp} dp = c_\phi dp \quad (4.7)$$
where \( c_\alpha = \frac{1}{\rho_\alpha} \frac{d\rho_\alpha}{dp} \) and \( c_\phi = \frac{d\phi}{dp} \) are the compressibility coefficients of the fluid phases and the rock, respectively, which are assumed to be constants.

The following vertically-integrated variables are defined

\[
\Phi \equiv \int_{\xi_B}^{\xi_T} \phi \, dx_3, \quad S_\alpha \equiv \frac{1}{\Phi} \int_{\xi_B}^{\xi_T} \phi s_\alpha \, dx_3, \quad U_{\alpha,\|} \equiv \int_{\xi_B}^{\xi_T} u_{\alpha,\|} \, dx_3, \quad (4.8a-c)
\]

\[
\Psi_{\alpha,\text{source/sink}} \equiv \int_{\xi_B}^{\xi_T} \psi_\alpha \, dx_3, \quad K \equiv \int_{\xi_B}^{\xi_T} k_{\|} \, dx_3, \quad \text{and} \quad \Lambda_\alpha \equiv K^{-1} \int_{\xi_B}^{\xi_T} k_{\|} \lambda_\alpha \, dx_3. \quad (4.9a-c)
\]

where subscript “\( \| \)” stands for the plane, and \( \lambda_\alpha \) is the mobility of phase \( \alpha \) which is the ratio of relative permeability to fluid viscosity.

The integrals of Equation (4.5) with the substitution of Equation (4.6) in the time derivative term yield

\[
\int_{\xi_B}^{\xi_T} \frac{\partial}{\partial t} (\rho_\alpha \phi s_\alpha) \, dx_3 = \rho_\alpha \frac{\partial}{\partial t} (\Phi S_\alpha) + \rho_\alpha c_\alpha \Phi S_\alpha \frac{\partial P_\alpha}{\partial t}, \quad (4.10)
\]

\[
\int_{\xi_B}^{\xi_T} \nabla \cdot (\rho_\alpha u_\alpha) \, dx_3 = \rho_\alpha \left[ \nabla \cdot U_{\alpha,\|} + \psi_\alpha^\alpha - \psi_\alpha^B \right], \quad (4.11)
\]

where we have used coarse-scale pressure, \( P_\alpha \), to represent the time rate of change of pressure along the \( x_3 \) direction. The coarse-scale pressure, \( P_\alpha \), is defined as the pressure of phase \( \alpha \) at a reference elevation, taken here to be the elevation of the bottom boundary of the formation, \( x_3 = \xi_B \), while \( \psi_\alpha^T \) and \( \psi_\alpha^B \) refer to the fluxes at the top and the bottom, respectively. It should be noted that lower-case variables represent fine-scale variables, while upper-case letters represent coarse-scale variables. The coarse-scale variables, which are defined in the context of vertical integration, can be obtained by either vertical averaging or sampling at one point in the vertical [Nordbotten and Celia, 2012], e.g. the coarse-scale
saturation, $S_\alpha$, and mobility, $\Lambda_\alpha$, are defined by vertical averaging, while the coarse-scale pressure, $P_\alpha$, is defined to be the reference pressure at the aquifer bottom.

Because of the VE assumption, the phase pressures are assumed to be hydrostatic:

$$p(x_1,x_2,x_3,t) = P_\alpha(x_1,x_2,t) + \rho_\alpha(g \cdot e_3)x_3,$$

where $e_3$ is the unit vector in $x_3$ direction (assumed to be positive upward).

With these definitions, Equation (4.5) yields the vertically-integrated mass balance equation

$$\frac{\partial (\Phi S_\alpha)}{\partial t} + c_\alpha \Phi S_\alpha \frac{\partial P_\alpha}{\partial t} + \nabla \parallel \cdot U_\parallel = \Psi_{\text{source/sink}} - \psi^\alpha_T + \psi^\alpha_B = \Psi.$$

The integrated flux in Equation (4.13) is

$$U_\parallel = -K \Lambda_\alpha \cdot (\nabla \parallel P_\alpha - \rho_\alpha G),$$

where $G = e_\parallel \cdot g + (g \cdot e_3)\nabla \parallel \zeta_B$, and $e_\parallel = (e_1, e_2)$.

Based on $k_{r,\alpha}(s_\alpha)$ and $p_{\text{cap}}(s_\alpha)$, the vertically-integrated mobility and capillary pressure can also be related to the vertically-integrated saturation algebraically, such that $\Lambda_\alpha(S_\alpha)$, $\hat{P}_c - P_b = P_{\text{cap}}(S_\alpha)$. The coarse-scale capillary pressure, $P_{\text{cap}}$, is a “pseudo capillary pressure”, which is defined as the difference between the coarse-scale pressures. Those pressures are, by definition, the phase pressures evaluated at the bottom of the formation; we use the notation $\hat{P}_c$ to denote the hydrostatic extension of the CO$_2$ phase pressure evaluated at the bottom of the formation, given that for many locations the CO$_2$ phase will not be present at the bottom boundary ($\zeta_B$). When neglecting capillary pressure, the functions $\Lambda_\alpha(S_\alpha)$ and $P_{\text{cap}}(S_\alpha)$ are linear and simple to derive. A detailed derivation of these two functions can be found in Nordbotten and Celia (2012). Although these functions become nonlinear when capillary pressure is included, they can be derived in an analogous way.
The vertically-integrated phase saturations also sum to unity.

\[ S_b + S_c = 1. \]  \hspace{1cm} (4.15)

By solving the vertically-integrated two-dimensional equations, we can compute the vertically-integrated saturation and one of the bottom phase pressures, both of which are coarse-scale variables. The pressure and saturation profiles along the vertical direction, which represent the fine scale of the problem, can then be reconstructed algebraically based on the VE assumption.

The applicability of VE models depends on the timescale of fluid segregation compared to the simulation time \( T \). If the segregation time is small relative to \( T \), then vertical equilibrium is usually a good approximation; otherwise the VE assumption is not applicable. The segregation time scale can be estimated from equation

\[ t_s \sim \frac{H \phi \mu_b}{k_{r,b,fine} k_z \Delta \rho g}, \]  \hspace{1cm} (4.16)

where \( H \) is formation height, \( \phi \) is rock porosity, \( \mu_b \) is brine viscosity, \( k_{r,b,fine} \) is the fine-scale relative permeability of brine, \( k_z \) is vertical permeability of the formation, \( \Delta \rho \) is the density difference between CO\(_2\) and brine, \( g \) is the acceleration of gravity.

To conceptually illustrate the process of reaching vertical equilibrium, we consider the injection of CO\(_2\) into an aquifer through a vertical well that fully penetrates the aquifer. Three schematic plots of the brine saturation profile at different times are shown in Figure 4.3. At early time, the brine is almost uniformly distributed in the vertical direction as CO\(_2\) invades horizontally along the fully penetrating vertical injection well. The CO\(_2\) then moves upward, driven by buoyancy, and brine simultaneously drains downward through the lighter CO\(_2\) driven by gravity. After a certain period of time, which is the time scale of segregation \( t_s \), CO\(_2\) and brine completely segregate with CO\(_2\) residing on top of brine. For simplicity, in Figure 4.3 we have neglected local capillary pressure. Therefore when
both CO$_2$ and brine reach vertical equilibrium, they form a macroscopic sharp interface, $\zeta_I$, as shown in Figure 4.3(c). If $t_s << T$, we can neglect the vertical redistribution process and simply assume CO$_2$ and brine have already segregated; this is the VE assumption. However, when $t_s$ is comparable or even larger than $T$ we have to include the vertical dynamics of CO$_2$ and brine in order to accurately predict CO$_2$ migration.

### 4.4 Multiscale algorithm — vertical dynamic reconstruction

The VE model is accurate and computationally efficient as long as the VE assumption is satisfied. However, such a simplified model will not be applicable when the timescale of fluid segregation is not small relative to the simulation time. In order to extend the applicability of vertically-integrated models, we present a multiscale method which relaxes the VE assumption and includes the vertical dynamics of CO$_2$ and brine, but still uses the vertically-integrated framework. We refer to this multiscale method as dynamic reconstruction, as opposed to static reconstruction in the VE model, because in the new approach flow dynamics are included in the vertical reconstruction. In this section, we first describe the dynamic reconstruction algorithm and then derive the equations for both the coarse and fine scales. We then present the numerical solution procedure that we have implemented.
Figure 4.4: Schematic description of the dynamic reconstruction algorithm: the coarse (horizontal) scale is a two-dimensional domain while the fine scale is represented by a series of one-dimensional (vertical) domains. The arrows indicate the flow of CO$_2$ and brine.

4.4.1 Algorithm overview

The dynamic reconstruction algorithm involves two scales: a coarse scale which is a vertically-integrated two-dimensional domain; and a fine scale that is a one-dimensional domain across the vertical extent of the formation (see Figure 4.4). The coarse (horizontal) scale is used to solve vertically-integrated equations for the coarse-scale pressure, $P_b(x_1,x_2,t)$. Given the solution for $P_b(x_1,x_2,t)$, the fine (vertical) scale is then solved for the phase saturation, using the fractional-flow form of the governing equation. By using no-flow boundary conditions along the top and bottom boundaries of the formation and horizontal fluxes (estimated from the solution for $P_b$) as local sources and sinks, the fractional-flow equation can be solved along any line in the direction ($\zeta_B < x_3 < \zeta_T$) for $s_c(x_1,x_2,x_3,t)$ as a one-dimensional problem. We then complete the calculations by using both $P_b(x_1,x_2,t)$ and $s_c(x_1,x_2,x_3,t)$ to analytically reconstruct the phase pressures along the $x_3$ direction.

4.4.2 Governing equations

The set of governing equations for the overall dynamic reconstruction algorithm has two parts: a vertically-integrated two-dimensional equation for the coarse-scale pressure, and
a set of one-dimensional equations for the fine scale. The coarse-scale equation is formed by summing the integrated mass balance equations for both fluid phases. This summed equation is analogous to the equation used in the VE models; the integrated mass balance equations are given already in Equation (4.13), and the summed equation takes the following form,

\[
(c_{\phi}H + c_{b}\Phi)S_{b}\frac{\partial P_{b}}{\partial t} + (c_{\phi}H + c_{c}\Phi S_{c})\frac{\partial P_{c}}{\partial t} + \Delta \cdot (U_{b,\|} + U_{c,\|}) = \Psi_{b} + \Psi_{c},
\]  

(4.17)

where the coarse-scale variables are as defined in Section 4.3. Note that the coarse-scale mobilities have to be numerically integrated from the fine-scale mobilities and they will hence differ from the VE case where it is obtained by an algebraic relation from the coarse-scale saturation. The definition of coarse-scale capillary pressure is also different from the VE algorithm; it is locally defined instead of being the “pseudo capillary pressure” as in the VE model.

To this point the procedure is almost identical to the vertical equilibrium approach, the differences being in the details of the coarse-scale coefficients as described above. However, as shown in Equation (4.12), the VE approach imposes a strict hydrostatic condition on both phase pressures, which serves to define the pressure structure used in the definition of integrated fluxes \( U_{b,\|} \) and \( U_{c,\|} \). The VE pressure distribution is inappropriate in the new algorithm, except in the limits where VE is applicable. Therefore, in the dynamic reconstruction, we use a more general pressure reconstruction. In the spirit of Equation (4.12), we write a generalized pressure function as

\[
p_{\alpha}(x_{1},x_{2},x_{3},t) = P_{\alpha}(x_{1},x_{2},t) + \pi_{\alpha}(x_{1},x_{2},x_{3},t).
\]  

(4.18)

In this equation, the function \( \pi_{\alpha} \) defines the vertical fine-scale reconstruction of the pressure field for phase \( \alpha \). Specific choices for this reconstruction function are discussed later in this section. With this reconstructed pressure, the integrated fluxes can be calculated
by computing the gradient in the $x_1$ and $x_2$ directions of the function $p_\alpha$. Equation (4.17) can then be solved for a coarse-scale pressure, which can be chosen as either $P_b$ or $P_c$ or any combination of these two pressures. $P_b$ is chosen in this chapter. Details of the numerical solution algorithm are given in Section 4.4.3.

In the fine-scale model, the phase mass balance equations are rearranged to focus on the vertical dynamics. The fine-scale mass balance for each phase can be written as follows,

$$
\frac{\partial (\phi s_\alpha)}{\partial t} + \frac{\partial u_{\alpha,3}}{\partial x_3} = \psi_\alpha - \nabla \parallel \cdot u_{\alpha,\parallel},
$$

(4.19)

where $u_{\alpha,3}$ is the flux of fluid phase $\alpha$ in the $x_3$ direction, and $u_{\alpha,\parallel}$ is the flux in the $(x_1, x_2)$ plane which will be estimated from the solution of Equation (4.17) and (4.18) by using Equation (4.20),

$$u_{\alpha,\parallel} = -k_{\parallel} \lambda_\alpha \left[ \nabla \parallel p_\alpha - \rho_\alpha (e_\parallel \cdot g) \right].
$$

(4.20)

Again as in the vertical equilibrium case, we assume “slight compressibility”, leading to

$$
\phi \frac{\partial s_\alpha}{\partial t} + (c_\phi + \phi c_\alpha) s_\alpha \frac{\partial p_\alpha}{\partial t} + \frac{\partial u_{\alpha,3}}{\partial x_3} = \psi_\alpha - \nabla \parallel \cdot u_{\alpha,\parallel}.
$$

(4.21)

Equation (4.21) is summed over the two phases, and the resulting equation is used to estimate the total flux, $u_{\text{tot},3}$ in the $x_3$ direction, where $u_{\text{tot},3} = u_{b,3} + u_{c,3}$. Given the total flux values in the $x_3$ direction, the vertical phase flux $u_{\alpha,3}$ can be calculated using the fractional flow form of Darcy’s Law, which takes the following form,

$$
u_{b,3} = f_b \left( u_{\text{tot},3} - k_3 \lambda_c \Delta \rho g + \lambda_c k_3 \frac{\partial p_{\text{cap}}}{\partial x_3} \right),
$$

(4.22a)

$$
u_{c,3} = f_c \left( u_{\text{tot},3} + k_3 \lambda_b \Delta \rho g - \lambda_b k_3 \frac{\partial p_{\text{cap}}}{\partial x_3} \right),
$$

(4.22b)

where $k_3$ is permeability in $x_3$ direction, and $f_\alpha$ is the fractional flow function, given by

$$f_\alpha = \frac{\lambda_\alpha}{\lambda_b + \lambda_c}.
$$

(4.23)
At this point, all the vertical and horizontal phase fluxes are known, allowing us to compute (reconstruct) the phase saturations using Equation (4.21).

Finally, we return to the issue of pressure reconstruction on the fine scale (Equation (4.18)). We seek a pressure reconstruction function that is simple to compute, is physically motivated, and produces the VE model at the appropriate limits. After experimenting with a number of choices, our current preferred choice is the following saturation-weighted pressure functions for the two phases:

\[
\frac{\partial p_c}{\partial x_3} = - (s_c \rho_c + s_b \rho_b) g + s_b \frac{\partial p^\text{cap}(s_b)}{\partial x_3},
\]

\[
\frac{\partial p_b}{\partial x_3} = - (s_c \rho_c + s_b \rho_b) g - s_c \frac{\partial p^\text{cap}(s_b)}{\partial x_3},
\]

From Equation (4.24), the function \( \pi_\alpha \) in Equation (4.18) can be derived. For example, when \( \alpha = b \), integration from the bottom of the formation yields

\[
p_b(x_1, x_2, x_3, t) = P_b(x_1, x_2, t) - \int_{x_3}^{\zeta_B} \left[ (s_c \rho_c + s_b \rho_b) g + s_c \frac{\partial p^\text{cap}(s_b)}{\partial x_3} \right] dx_3.
\]

It should be noted that the reconstructed fine-scale pressure is only used to compute horizontal fine-scale fluxes, and is not directly used in the vertical flux calculation. Thus the appropriateness of the pressure reconstruction only depends on how well it captures the horizontal fine-scale fluxes. There are three forces that drive the horizontal flow: the viscous force, capillary pressure, and buoyancy. Different forces become dominant in different regimes or periods. For the regime that is close to the injection well or before \( \text{CO}_2 \) and brine segregate, viscous forces dominate. For the regime that is far from the injection well, or after \( \text{CO}_2 \) and brine segregate, capillary pressure and gravity forces become dominant. The pressure reconstruction should be able to capture the evolution of the dominant forces. Any reconstruction that has the coarse-scale pressure included can approximately capture the viscous forces when viscous forces are dominant, while the saturation-weighted
hydrostatic pressure profile is currently the only reconstruction we have developed that not only accounts for the viscous forces, but also captures the capillary pressure and buoyancy when these two forces become dominant. Other options could be chosen, for example, instead of using the fine-scale reconstructed pressure field, the coarse-scale horizontal pressure gradient can be used to compute the fine-scale fluxes (that is, apply the coarse pressure gradient along the entire vertical). This option gives good results when CO$_2$ and brine are not segregated, meaning it captures the viscous forces well, but it induces significant errors when CO$_2$ and brine segregate and reach vertical equilibrium. This is simply because when CO$_2$ and brine are in equilibrium, fine-scale pressure gradient is different from the coarse-scale pressure gradient and that difference is largely due to capillary pressure and buoyant force. Other choices may be explored for the pressure reconstruction, but our results to date indicate that the saturation-weighted reconstruction gives good results.

4.4.3 Numerical solution procedure

To solve the dynamic reconstruction model numerically we discretize space by using a standard cell-centered finite-volume method. For the time discretization we use a scheme analogous to the implicit pressure and explicit saturation (IMPES) method: an implicit treatment of the pressure at the coarse scale and an explicit treatment of saturation at the fine-scale decouples the two scales. We hence are able to first solve the coarse-scale pressure implicitly and then calculate the fine-scale saturations explicitly. Details of the algorithm implementation are presented in this section. For the sake of clarity, we use continuous operators in space in our exposition.
The time-discrete version of Equation (4.17) with implicit brine pressure \( P_b \) and explicit treatment of saturations is given by

\[
(c_\phi H + c_b \Phi_S b^n + c_c \Phi_S c^n) \frac{P_b^{n+1} - P_b^n}{\Delta t} + (c_\phi H + c_c \Phi_S c^n) \frac{P_{\text{cap}}^{n} - P_{\text{cap},n-1}}{\Delta t} - \nabla \cdot \{ K \left[ (\Lambda_b^n + \Lambda_c^n) \cdot \nabla ||P_b^{n+1} + \Lambda_c^n \nabla P_{\text{cap},n} - (\Lambda_b^n \rho_b + \Lambda_c^n \rho_c)(e\parallel \cdot g) \right] \\
+ \int_{\zeta_3} \kappa_{\parallel} (\lambda_b^n \Delta || \pi_b^n + \lambda_c^n \nabla || \pi_c^n) dx_3 \} = \Psi_{b,n+1} + \Psi_{c,n+1}.
\] (4.26)

where superscript \( n \) stands for the discrete time level \( t^n \) and \( n + 1 \) stands for \( t^{n+1} \). This is a linear equation for the coarse-scale pressure \( P_b^{n+1} \) at time \( t^{n+1} \) that can be solved by a sparse matrix solver.

For the fine-scale transport of the saturations using Equation (4.21), we first calculate the horizontal phase fluxes as follows

\[
u^{n+1,*}_{n+1,\parallel} = -k_{\parallel} \lambda_{n} \left[ \nabla || P_{\alpha,n+1,*} - \rho_{\alpha} (e\parallel \cdot g) \right].
\] (4.27)

where \( P_{\alpha,n+1,*}(x_1, x_2, x_3) = P_{\alpha}^{n+1}(x_1 + x_2) + \pi_{\alpha}^{n}(x_1, x_2, x_3) \), and the superscript * denotes that the variable is an approximation at time \( t^{n+1} \).

The horizontal total flux \( u^{n+1,*}_{\text{tot,\parallel}} = u^{n+1,*}_{b,\parallel} + u^{n+1,*}_{c,\parallel} \) is then used to calculate the vertical total flux from the time-discrete version of Equation (4.21) summed over the two phases, that is

\[
\frac{\partial u^{n+1,*}_{\text{tot,3}}}{\partial x_3} = -\Delta || u^{n+1,*}_{\text{tot,\parallel}} + \psi_b^{n+1} + \psi_c^{n+1} - (c_\phi + \phi_c) s_{c}^{n} \frac{p_{b}^{n+1,*} - P_b^n}{\Delta t} - (c_\phi + \phi_c) s_{c}^{n} \frac{p_{c}^{n+1,*} - P_c^n}{\Delta t}. (4.28)
\]

With the vertical total flux \( u^{n+1,*}_{\text{tot,3}} \) and no-flow boundary conditions at the top and bottom of the formation, we obtain the phase fluxes with the time-discrete version of Equa-
Given the initial value of pressure $p^0$ and saturation $s^0$:

**For all** discrete time steps $n = 0, 1, ..., N$ do

1. Compute $\lambda^n_{\alpha}$ and $\Lambda^n_{\alpha}$, solve for $P^n_{\beta}$; compute $u^{n+1,*}_{\alpha,||}$ and $u^{n+1,*}_{\text{tot}}$;
2. Assume $p^{n+1,*}_{\alpha} = P^n_{\alpha} + \mathbf{\pi}^n_{\alpha}$, compute $u^{n+1,*}_{\alpha,||}$ and $u^{n+1,*}_{\text{tot}}$;
3. Compute $s^{n+1}_{\alpha}$, analytically reconstruct $p^{n+1}_{\alpha}$.

**End for**

Table 4.1: Numerical solution procedure for the dynamic reconstruction algorithm.

---

The solution procedure is summarized in Table 4.1.
4.5 Results

In this section, we present results from the dynamic reconstruction model and compare them with results from two other models: a full multi-dimensional model and a VE model. For simplicity, we compare them in a two-dimensional cross-sectional domain so that the problem setup only has one horizontal dimension and one vertical dimension. The full multi-dimensional model is therefore a two-dimensional simulator, which solves the full equations using an IMPES method (Doster et al. 2013). For most of the test cases, we neglect capillary pressure, so that the VE model is a sharp-interface model. This allows for easy visual comparison of the results. Also, we neglect compressibility for simplicity.

Two test scenarios have been designed (Figure 4.5). The first scenario involves injection through a vertical, fully penetrating well, while the second scenario involves injection from a location at the bottom of the formation. In each scenario, we will present CO$_2$ plume comparisons for both early times (1 ∼ 5 years) and later time (50 years). In the first scenario, we neglect capillary pressure and study two different values of permeability. We expect that the time scale of fluid segregation for the larger permeability (100 mD) is small so that it is consistent with the VE assumption, while with the lower permeability (10 mD) the fluids take a longer time to segregate in which case the VE assumption may be invalid. In the second scenario, we keep the permeability fixed at 10 mD and study the performance of the dynamic reconstruction model both with and without capillary pressure.

The problem setup for both scenarios is shown in Figure 4.5. Top and bottom boundaries are no-flow. Along the left boundary, CO$_2$ is injected from a well at a constant flow rate. The well spans the entire thickness of the formation in the fully penetrating case, and only the bottom 1 meter in the partially penetrating case. Along the right boundary, a flux boundary condition is imposed where we extract, uniformly along the vertical direction, the same mass of fluid as we inject on the left side. The formation is 50 m thick, and the domain size in the x direction depends on different simulation times: a shorter length is chosen for early-time simulations to allow use of fine grid spacing. For early-time simula-
Figure 4.5: Problem setup for the numerical experiments, (a) fully penetrating case, (b) partially penetrating case.

In this section, two cases with fully penetrating injection wells will be presented. The first case involves a relatively low permeable formation with permeability of 10 mD, while the second case has a higher permeability of 100 mD. The time scale of vertical fluid segregation is larger in the low permeability case than in the high permeability case, so that the low permeability case is less favorable for VE models.

In Figures 4.6, we present comparisons for the case with a permeability of 10 mD. Different rows show results for different simulation times. The top two rows show the CO$_2$ plumes for the three models for early simulation times, which we take to be the first 5 years after injection begins; the bottom row shows the CO$_2$ plumes for late times, which we take...
Figure 4.6: A comparison of the CO$_2$ plumes for the three models under a fully penetrating injection scenario, with the permeability of the formation being 10 mD and capillarity neglected. The three rows show results at $t = 1$ year, $t = 5$ years and $t = 50$ years, respectively. Note the scale on the $x$-axis is ten times larger in the third row. The left and center columns show the predicted CO$_2$ plumes using the dynamic reconstruction model and the full two-dimensional model, respectively. The color indicates the magnitude of CO$_2$ saturation, while the superimposed red (white for the third row) dashed line shows the CO$_2$-brine interface from the VE model. The right column shows the location of the CO$_2$ invasion front for all three models.
to be 50 years. We show results for the spatial distribution of the CO$_2$ (left and center columns) as well as a comparison of the CO$_2$ invasion front location for all three models in the right column. From the comparison, we can see that the dynamic reconstruction model is very close to the full two-dimensional model both in terms of the CO$_2$ distribution and the CO$_2$ invasion front. The CO$_2$ invasion front is defined as the transition from grid cells with CO$_2$ saturation greater than 1% to neighbor cells with saturation less than 1%. The red (white for the third row) dashed line in the left and center panels represent the CO$_2$-brine interface from the VE model. In the VE model, CO$_2$ saturation above the interface is 1 and below it is 0 (no residual saturation considered here). The CO$_2$ plume from the VE model is different from the other two models and we can see that it tends to overestimate the outer-most extent (or tip) of the CO$_2$ front. In fact, the tip of the CO$_2$ plume has traveled about twice as far as for the VE model, and the shape of the invading fronts remains different even though the fluids are strongly segregated after 50 years. Overall, the dynamic reconstruction model matches the full two-dimensional model very well, while the VE model is significantly different for all times.

The CO$_2$ plume comparison for the case with 100 mD is shown in Figure 4.7. For early simulation times, the three models are all very close (see top two rows of Figure 4.7). If we look at the longer simulation times, they become even closer (see bottom row of Figure 4.7). The VE assumption appears to work well in this case, and we can see that the three models give similar results, although the VE model still overestimates the tip location.

### 4.5.2 CO$_2$ plume comparison for a partially penetrating injection well

The second injection scenario is injection through a partially penetrating well, as illustrated in Figure 4.5(b). In this case, CO$_2$ is injected through the bottom 1m of the aquifer, and the total injection rate is the same as for the fully penetrating case and hence the CO$_2$ is injected at higher velocity and across a steeper pressure gradient. Because more vertical pressure driven flow is involved, especially close to the injection well, this is a stronger test
Figure 4.7: A comparison of the CO$_2$ plumes for the three models under a fully penetrat-
ing injection scenario, with permeability of the formation being 100 mD and capillarity
neglected. The three rows show results at $t = 1$ year, $t = 5$ years and $t = 50$ years, respec-
tively. The left and center columns show the predicted CO$_2$ plumes using the dynamic
reconstruction model and the full two-dimensional model, respectively. The color indi-
cates the magnitude of CO$_2$ saturation, while the superimposed white dashed line shows
the CO$_2$-brine interface from the VE model. The right column shows the location of the
CO$_2$ invasion front for all three models.
Figure 4.8: A comparison of the CO$_2$ plumes for the three models under a partially penetrating injection scenario, with permeability of the formation being 10 mD and capillarity neglected. The three rows show results at $t =$ 1 year, $t =$ 5 years and $t =$ 50 years, respectively. The left and center columns show the predicted CO$_2$ plumes using the dynamic reconstruction model and the full two-dimensional model, respectively. The color indicates the magnitude of CO$_2$ saturation, while the superimposed red (white for the third row) dashed line shows the CO$_2$-brine interface from the VE model. The right column shows the location of the CO$_2$ invasion front for all three models.

of the dynamic reconstruction model, in particular the assumption of a saturation-weighted hydrostatic pressure profile in the pressure reconstruction. Here, we show the results for the case with relatively low permeability (10 mD), since this is the more challenging case for the dynamic reconstruction model. In the 100 mD case (not shown here), we observe very good agreement of the dynamic reconstruction and the full two-dimensional model and all three models are close, similar to what was observed in the fully penetrating case with permeability of 100 mD.
The comparison of the three models for the partially penetrating scenario without capillary pressure is shown in Figure 4.8. Again, the top two rows are for early simulation times and the bottom row is for late simulation time. Despite injecting from the bottom of the aquifer, the results show that the dynamic reconstruction model is still close to the full two-dimensional model. Even the non-monotonic saturation distribution along horizontal cross-sections in the middle of the aquifer (see center row of Figure 4.8) is captured well. The only significant difference occurs for the earliest time (i.e. after 1 year injection), where we observe that the dynamic reconstruction model has more CO$_2$ at the top of the aquifer and that the CO$_2$ at the top moves slightly further away from the left boundary, as compared with the full two-dimensional model. But, in that case, we can see that the VE model gives much worse results than the dynamic reconstruction model: all of the CO$_2$ accumulates to the top part of the aquifer due to the VE assumption.

Finally, a CO$_2$ plume comparison of the three models for a partially penetrating injection scenario with capillary pressure taken into account is shown in Figure 4.9. Similar to the case without capillary pressure, the dynamic reconstruction shows very good agreement with the full two-dimensional model except at the earliest time (i.e. after 1 year injection). But, again, the VE model gives much worse results than the dynamic reconstruction model in that case. We should note that although the VE model is still quite different from the other two models, it gives better results compared to the case without capillary pressure. In particular, the VE model tends to overestimate the outer-most extent of the CO$_2$ plume less when capillary pressure is included.

4.6 Discussion

The model comparisons show that the dynamic reconstruction model agrees very well with the full two-dimensional model for the considered injection scenarios: an injection with a fully penetrating well into a low or high permeable formation as well as an injection with a
Figure 4.9: A comparison of the CO$_2$ plumes for three models under a partially penetrating injection scenario, with the permeability of the formation being 10 mD and capillary pressure included. The three rows show results at $t = 1$ year, $t = 5$ years and $t = 50$ years, respectively. The left, center and right columns show the predicted CO$_2$ plumes using the dynamic reconstruction model, the full two-dimensional model and the vertical equilibrium model, respectively. The color indicates the magnitude of CO$_2$ saturation.

partially penetrating well with or without capillary pressure. In the fully penetrating injection scenario, the dynamic reconstruction model shows excellent agreement with the full two-dimensional model for all simulation times. For the partially penetrating injection scenario there is some difference between the CO$_2$ plumes from the dynamic reconstruction model and the full two-dimensional model at early times (i.e. after 1 year injection). This is not surprising, based on our pressure reconstruction method. The reconstructed pressure profile is not used directly in the algorithm, instead only the horizontal pressure gradient is used to compute horizontal fluxes. Such an approximation works very well for the fully penetrating case even if the pressure profile is not hydrostatic. For the fully penetrating
well the horizontal pressure gradient is almost uniformly distributed along the vertical, so that the horizontal pressure gradient calculated from the saturation weighted hydrostatic pressure profile, which is ultimately based on the pressure gradient at the bottom of the formation, is a good approximation. However, for the partially penetrating case, especially close to the well, pressure driven flow in the vertical direction is more pronounced leading to a less uniform horizontal pressure gradient distribution. In fact, the horizontal pressure gradient at the top may differ significantly from the gradient at the bottom close to the well. Therefore, the reconstructed pressure profile in the dynamic reconstruction model tends to overestimate the horizontal flux at the top of the aquifer, which leads to overestimation of the vertical flux as well. As such, the dynamic reconstruction model overestimates the amount of CO$_2$ at the top and the location of the tip of the CO$_2$ plume compared with the full two-dimensional model, especially at early times. It should be noted that, from a regulatory perspective the algorithm can thus be assumed to be conservative, as the CO$_2$ plume area would be overestimated. However, at later times, even after only 5 years, there is good agreement between the dynamic reconstruction model and the full two-dimensional model. This is because further away from the well the horizontal pressure gradient becomes more uniform along the vertical direction and this renders our pressure approximation more reasonable. Overall, we observe that the dynamic reconstruction appears to give remarkably good agreement with the full two-dimensional model, even for the partially penetrating case, especially at later times.

The dynamic reconstruction model naturally maintains much of the computational efficiency of the VE models because it still uses the vertically-integrated framework. The pressure solution, which usually requires the most computational effort in an IMPES-type method, is only solved in two dimensions in the coarse-scale model. The transport solution is decoupled into a one-dimensional countercurrent flow in the vertical and a two-dimensional transport in the horizontal. Therefore we do solve the transport in three dimensions (explicitly), which in the case of fast vertical segregation may be constrained by
a CFL condition that is significantly stricter than the purely horizontal two-dimensional transport in VE models. This may be remedied by using smaller time steps in the transport calculation compared to the coarse-scale pressure solution. The higher cost of the dynamic reconstruction model also reflects that before the fluids segregate in the vertical, some computational effort must be spent to resolve the vertical flow. Because of the decoupling between the coarse scale and fine scale, we observe the grid sizes cannot be chosen independently. Smaller ratios of $\Delta z/\Delta x$ give better agreement with the full two-dimensional simulation; based on numerical experimentation, we choose the ratio $\Delta z/\Delta x$ less than unity, often on the order of 0.1. However, we note that since the physical system of CO$_2$ storage usually has orders of magnitude larger extent in the horizontal than in the vertical direction, the spatial discretization naturally leads to a small grid size ratio in order to be computationally practical. In terms of computational efficiency, despite inclusion of more physics, the dynamic reconstruction model only takes about twice of the computational time compared to the VE model per time step even if 50 grid cells are placed along the vertical. We should note that the time step of the dynamic reconstruction model may be restricted by the fine-scale calculation, but in that case, a different (larger) time step could be chosen for the coarse scale. By comparison with the full two-dimensional model, even if these two algorithms are implemented in different programming languages and using different linear system solvers, we observe that the dynamic reconstruction model is at least one order of magnitude faster for most cases. Overall, this implies that the dynamic reconstruction model captures more physics than the VE models while still maintaining much of the computational advantages over full multi-dimensional models.

Because the purpose of this chapter is to introduce the new dynamic reconstruction algorithm, we have used relatively simple example problems to demonstrate the concept and to show that the algorithm appears to give significant improvements compared to the VE model while retaining many of its attractive features. All of the example problems involve homogeneous, horizontal, isotropic formations with uniform thickness involving
two immiscible fluid phases. The design of the algorithm does not explicitly rely on these simplifications. Thus, we expect that inclusion of material heterogeneities, geometric complexities, and phase interactions including dissolution and miscible transport is possible within our general framework. However, we have not implemented those extensions, so their efficacy remains to be studied.

4.7 Conclusion

A novel multiscale method for modeling CO$_2$ storage has been presented in this chapter, based on vertically-integrated equations coupled with a dynamic reconstruction of saturation and pressure in the vertical direction. This differs from the usual vertically integrated models, which assume vertical equilibrium and therefore do not include any vertical flow dynamics. For the example problems studied, the new model shows excellent agreement with full multidimensional models, and shows significant improvements over Vertical Equilibrium (VE) models for cases when vertical equilibrium is not an appropriate assumption. The new model also matches the VE results in the limit of very fast segregation times, which are the cases for which VE is applicable. Overall, the dynamic reconstruction model provides a new multiscale framework for large-scale CO$_2$ storage problems which extends the scope of applicability of vertically-integrated models. Extensions to include additional fine-scale physics, such as vertical heterogeneity and fluid solubility, should also be possible although we have not yet explored these in any depth.

The dynamic reconstruction model maintains much of the computational advantages of the VE model and therefore requires much less computational effort compared to full multi-dimensional models. The ability to capture more physics while still maintaining a low level of computational effort makes these dynamic reconstruction models feasible for computational studies of large-scale CO$_2$ storage systems where the vertical dynamics of CO$_2$ and brine are important.
Chapter 5

A Multi-layer Dynamic Reconstruction Model for CO$_2$ Sequestration in Layered Geologic Formations

This chapter is adopted from the publication:


5.1 Abstract

Efficient computational models are desirable for simulation of large-scale geologic CO$_2$ sequestration. Vertically-integrated models, which take advantage of dimension reduction, offer one type of computationally efficient model. The dimension reduction is usually achieved by vertical integration based on the vertical equilibrium (VE) assumption, which assumes that CO$_2$ and brine segregate rapidly in the vertical due to strong buoyancy and quickly reach pressure equilibrium. However, the validity of the VE assumption requires
small time scales of fluid segregation, which may not always be fulfilled, especially for heterogeneous geologic formations with low vertical permeability. Recently, Guo et al. (2014a) developed a multiscale vertically-integrated model, referred to as the dynamic reconstruction (DR) model, that relaxes the VE assumption by including the vertical two-phase flow dynamics of CO$_2$ and brine as fine-scale one-dimensional problems in the vertical direction. Although the VE assumption can be relaxed, that model was limited to homogeneous geologic formations. Here, we extend the multiscale algorithm of Guo et al. (2014a) for layered heterogeneous formations, which is of much more practical interest for saline aquifers in sedimentary basins. We develop a new coarse-scale pressure equation to couple the different coarse-scale (vertically-integrated) layers, and use the fine-scale dynamic reconstruction algorithm in Guo et al. (2014a) within each individual layer. Together, these form a multiscale multilayer dynamic reconstruction algorithm. Simulation results of the CO$_2$ plume from the new model are in excellent agreement with full three-dimensional models, with the new algorithm being much more computationally efficient than conventional full three-dimensional models.

5.2 Introduction

Geologic carbon sequestration (GCS) has been proposed and demonstrated as a feasible technology to reduce anthropogenic carbon dioxide (CO$_2$) emissions into the atmosphere, as part of the framework of global warming mitigation technologies (Pacala and Socolow, 2004; IPCC, 2005; Michael et al., 2010; Celia et al., 2015). For GCS to be an effective carbon mitigation strategy, several engineering questions have to be answered related to CO$_2$ storage capacity, CO$_2$ injectivity, and containment within the geologic storage unit. Depending on the physical processes that are important over the length and time scale associated with specific questions, mathematical models with different levels of complexity can be developed (Nordbotten and Celia, 2012; Bandilla et al., 2015; Celia et al., 2015).
One feature of the GCS system is that the large density difference between CO$_2$ and the resident brine leads to strong buoyant segregation. If the time scale associated with the fluid segregation is small relative to the time scale associated with the overall simulation time, the two fluid phases may be assumed to always be segregated and to be in pressure equilibrium in the vertical direction. With such a vertical equilibrium (VE) assumption, the general three-dimensional two-phase flow equations can be simplified to a set of two-dimensional equations by vertical integration (e.g., Bear, 1972; Lake, 1989; Wu et al., 1994; Gasda et al., 2009; Nordbotten and Celia, 2012), which can even be further simplified to one-dimensional equations by assuming symmetric flows (see e.g., Huppert and Woods, 1995; Nordbotten and Celia, 2006; Hesse et al., 2008; MacMinn et al., 2010; Pegler et al., 2014; Zheng et al., 2015a). The dimension reduction decreases computational effort significantly, which makes the VE models very computationally efficient. However, the applicability of vertically-integrated models depends strongly on the vertical equilibrium assumption, which may not always be appropriate, especially for geologic formations with relatively low permeability or heterogeneous formations with a wide range of permeabilities, where it takes significant time for the buoyant segregation to occur (Court et al., 2012).

Recently, a new type of vertically-integrated model that does not rely on the VE assumption has been developed (Guo et al., 2014a). This new model casts the governing equations into two scales: a set of vertically-integrated equations in the horizontal domain (coarse scale) and a set of one-dimensional equations resolved in the vertical domain defined over the thickness of the formation (fine scale). Similar to the conventional vertically-integrated models, the new model also solves a set of vertically-integrated equations (on the coarse scale). However, in contrast to conventional VE models, the new model solves a set of one-dimensional equations in the vertical (fine scale) for the two-phase flow dynamics of CO$_2$ and brine instead of assuming that the two fluid phases have fully segregated. This new model is referred to as the dynamic reconstruction (DR) model, in the sense that
it is a vertically-integrated model that dynamically reconstructs the vertical fluid distribution at every time step (as opposed to VE models that use equilibrium fluid distribution). The dynamic reconstruction model maintains the computational advantages of the vertical equilibrium models because the pressure equation is only solved on the coarse scale, and only marginal additional computational effort is required to solve the one-dimensional problems for the vertical dynamics of CO$_2$ and brine \cite{Guo et al. 2014a}. Being able to capture vertical dynamics of CO$_2$ and brine while maintaining much of the computational advantages of the VE models, the dynamic reconstruction model provides an intermediate model choice between the VE model and full three-dimensional models.

Although the dynamic reconstruction model in \cite{Guo et al. 2014a} can capture vertical dynamics of CO$_2$ and brine, it currently only applies to a single homogeneous formation. Here, we extend this model to include spatial heterogeneity in the vertical dimension. Specifically, we focus on layered heterogeneity, which is a typical type of heterogeneity for saline aquifers due to their geologic deposition history. The geologic formation with layered heterogeneity has multiple layers, each of which may have different geologic properties, while each of these layers is homogeneous. Such layered systems are common geologic structures in the sedimentary aquifers \cite{Nicot 2008, Birkholzer et al. 2009, Zhou et al. 2010, Cihan et al. 2011, Bandilla et al. 2012, Doughty and Freifeld 2013}, which is a major type of target formations for CO$_2$ sequestration \cite{IPCC 2005, Nordbotten and Celia 2012, Birkholzer et al. 2015}. For these layered systems, we need to model CO$_2$ migration within and through the layers. We use the same algorithm as that was used in \cite{Guo et al. 2014a} for CO$_2$ migration within each individual layer, while for CO$_2$ migration through the layers, we develop a coarse-scale pressure equation that computes the vertical fluxes of CO$_2$ and brine between the layers. These fluxes are computed by using the vertical coarse-scale pressure gradient and the fine-scale information (fluid mobilities and geologic properties) between the centers of the two layers, leading to an effective coarse-scale Darcy type flux equation in the vertical direction. The coupling through the coarse-scale
pressure equations, together with the dynamic reconstruction, form a multilayer dynamic reconstruction model which is able to model CO₂ migration in a geologic formation with layered heterogeneity.

In structuring this chapter, we first present the general governing equations of two-phase flow, after which we present the mathematical formulations of the multilayer dynamic reconstruction model and the associated numerical scheme we use. This is followed by a comparison of the new model to a conventional three-dimensional simulator, based on modeling results for both an idealized two-layer formation and a more realistic multiple-layer formation with parameters based on the Mt Simon formation of the Illinois Basin. Then we discuss advantages and future directions of the new model. We close the chapter with several concluding remarks.

5.3 Mathematical and numerical models

For a geologic formation with multiple lateral layers, we cast the entire system into two scales (see Figure 5.1): a (horizontal) coarse-scale that corresponds to the geologic layers with different geologic properties, and a (vertical) fine-scale that represents the thickness of each of those layers. On the coarse scale, we integrate the three-dimensional equations within each layer in the vertical and obtain a coarse-scale pressure equation, where the coarse-scale pressure is defined as the pressure in the middle of each layer along the vertical direction. To couple all the layers, we develop a multilayer coarse-scale pressure equation that couples the coarse-scale pressure equation at each layer. On the fine scale, we solve the transport equation for the fine-scale saturation and pressure along the vertical columns with the dynamic reconstruction algorithm in Guo et al. (2014a). In the following subsections, we derive the multilayer coarse-scale pressure equation for the coarse-scale layers and briefly review the fine-scale dynamic reconstruction algorithm. Following that, we present the numerical schemes to solve this multiscale framework.
Figure 5.1: Schematic of the multiscale multilayer dynamic reconstruction algorithm, with three layers as an example. The fine-scale columns belong to the coarse-scale layer, and here we take the columns of the second layer ($Z_2$) as an example. The arrows in the columns represent the fluxes from layer $Z_2$ to layer $Z_3$ and from layer $Z_1$ to layer $Z_2$ at the layer boundaries.
5.3.1 Full three-dimensional equations

We treat the CO$_2$ injection system as a two-phase flow problem, neglecting mutual miscibility between the two fluid phases. Note that the multiscale framework in this chapter in principle can be extended to include component transport, although we have not explored it in detail. We assume immiscibility between the two fluid phases, in part because the mutual solubility between CO$_2$ and brine is small, up to a few percents \cite{Nordbotten2012}, and also because this chapter focuses on the CO$_2$ injection period which has a time scale that is short relative to the time scale for convective mixing of CO$_2$ and brine due to CO$_2$ dissolution \cite{Emami-Meybodi2015}. Before proceeding to the multiscale algorithms, we first go through the full three-dimensional equations for two-phase flow in porous media as a basis for the development of the multiscale equations.

The general governing equations for two-phase flow in porous media consist of a mass balance equation and an equation of the extended Darcy’s law for each of the fluid phases, as shown in Equation (5.1) and Equation (5.2), respectively

\[
\frac{\partial}{\partial t} (\rho_\alpha \phi s_\alpha) + \nabla \cdot (\rho_\alpha u_\alpha) = \rho_\alpha \psi_\alpha, \tag{5.1}
\]

\[
u_\alpha = -\frac{k_{r,\alpha} k}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g), \tag{5.2}
\]

where $\alpha = b$ or $c$, representing the fluid phase of brine ($b$) or CO$_2$ ($c$), $\rho_\alpha$ is fluid density, $s_\alpha$ is phase saturation, $\phi$ is porosity of the geologic porous media, $u_\alpha$ is the volumetric Darcy velocity, and $\psi_\alpha$ is a source term (or sink term if negative);

where $k_{r,\alpha}$ is relative permeability, $k$ is the permeability tensor of the geologic formation, $\mu_\alpha$ is viscosity, $p_\alpha$ is phase pressure, and $g$ is gravity acceleration. The relative permeability $k_{r,\alpha}$ is commonly parameterized as a function of phase saturation, that is $k_{r,\alpha} = k_{r,\alpha}(s_\alpha)$. The two phase pressures are related by the capillary pressure, which is also usually taken
as an empirical function of phase saturation

\[ p_c - p_b = \rho_{\text{cap}}(s_\alpha). \]  

(5.3)

Finally, the pore space has to be filled up with the two fluid phases, so the phase saturations should sum to unity

\[ s_b + s_c = 1. \]  

(5.4)

5.3.2 Coarse-scale pressure equation of the coupled layers

In a multilayer geologic formation, the layers are hydraulically connected. Therefore, the coarse-scale individual layer should be coupled with the neighbor layers. That is, the coarse-scale pressure equation will be three-dimensional, where the coarse-scale vertical dimension represents the number of coarse-scale layers. We proceed to derive the coarse-scale pressure equation in two steps. First, we write a vertically-integrated mass balance equation for each layer, then we derive an equation for the total fluxes between the layers that couple the coarse-scale pressures of the two layers. The end result is a multilayer pressure equation that couples coarse-scale pressures in the entire formation. Details of the standard procedure of vertical integration for two-phase flow equations can be found in the literature (e.g., Nordbotten and Dahle, 2011; Nordbotten and Celia, 2012; Gasda et al., 2012a). An integration procedure with respect to general pressure profiles (without assuming vertical equilibrium of the fluid phases) can be found in Guo et al. (2014a).

Following Guo et al. (2014a), the pressure profile in an individual layer can be represented as a reference pressure plus the deviation from the reference pressure, shown in Equation (5.5)

\[ p_\alpha(x,y,z,t) = P_\alpha(x,y,t) + \pi_\alpha(x,y,z,t), \]  

(5.5)
where \( p_\alpha(x,y,z,t) \) is the fine-scale phase pressure at point \((x,y,z)\) and \( P_\alpha(x,y,t) \) is the pressure at a reference point which we define as the coarse-scale pressure, and \( \pi_\alpha(x,y,z,t) \) is the deviation of the fine-scale phase pressure at \((x,y)\) from the reference pressure. The axis of \((x,y)\) is chosen to be in the plane of the general lateral direction of the formation, and the \( z \) axis is the direction orthogonal to the \((x,y)\) axis (assuming upward positive). Note that the reference pressure can be chosen at any point along the \( z \) direction. Here we choose the reference pressure to be in the center of the layer (along the \( z \) axis).

Integrating Equation (5.1) in the \( z \) direction from \( z = \zeta_B \) (bottom of the layer) to \( z = \zeta_T \) (top of the layer) and suming over the two fluid phases, we obtain (Guo et al., 2014a)

\[
(c_\phi H + c_b \Phi) S_b \frac{\partial P_b}{\partial t} + (c_\phi H + c_c \Phi) S_c \frac{\partial P_c}{\partial t} + \nabla \parallel \cdot (U_b + U_c) = \Psi^b + \Psi^c - u_{\text{tot},z}|_{\zeta_T} + u_{\text{tot},z}|_{\zeta_B},
\]

(5.6)

where \( H \) is the thickness of the geologic layer; \( c_\phi, c_b \) and \( c_c \) are the compressibility coefficients (assumed to be constants) of the porous medium, brine, and \( \text{CO}_2 \), respectively; the “parallel to” subscript \( \parallel \) represents the \((x,y)\) plane and \( \nabla \parallel = \frac{\partial}{\partial x} e_x + \frac{\partial}{\partial y} e_y \), where \( e_x \) and \( e_y \) are unit vectors in \( x \) and \( y \) direction; \( u_{\text{tot},z}|_{\zeta_T} \) and \( u_{\text{tot},z}|_{\zeta_B} \) denote the total fluxes (sum of the \( \text{CO}_2 \) and brine fluxes) at the top and the bottom of the layer respectively; the vertically-integrated saturations are defined as \( S_\alpha \equiv 1/\Phi \int_{\zeta_B}^{\zeta_T} \phi s_\alpha \, dz \) with \( \Phi \equiv \int_{\zeta_B}^{\zeta_T} \phi \, dz \); and \( \Psi^\alpha \) is the vertically-integrated source term of \( \alpha \) phase. The vertically-integrated horizontal fluxes have the following expressions

\[
U_\alpha = -K_\parallel \Lambda_\alpha \cdot (\nabla \parallel P_\alpha - \rho_\alpha G) - \int_{\zeta_B}^{\zeta_T} k_\parallel \lambda_\alpha \nabla \parallel \pi_\alpha \, dz,
\]

(5.7)

where \( G \equiv e_\parallel \cdot g + (g \cdot e_z) \nabla \parallel \zeta_B \) and \( e_\parallel = (e_x, e_y)^T \); \( K_\parallel \equiv \int_{\zeta_B}^{\zeta_T} k_\parallel \, dz \); \( \lambda_\alpha = \frac{k_\parallel \alpha}{\mu_\alpha} \), is the mobility of fluid phase \( \alpha \); \( \Lambda_\alpha \equiv K_\parallel^{-1} \int_{\zeta_B}^{\zeta_T} k_\parallel \lambda_\alpha \, dz \), is the vertically-integrated mobility of fluid phase \( \alpha \).

The total fluxes at the top \((u_{\text{tot},z}|_{\zeta_T})\) and the bottom \((u_{\text{tot},z}|_{\zeta_B})\) in Equation (5.6) are zero in the single layer dynamic reconstruction model in Guo et al. (2014a). Thus, Equa-
Figure 5.2: An illustration of the total flux between two layers. Here, we take the layers $j$ and $j+1$ as an example. $\zeta_j$, $\zeta_{j+1}$ and $\zeta_{j+2}$ are the interlayer boundaries. The light green highlighted areas are two (neighbor) vertical columns of layer $j$ and $j+1$, which have $P_{b,j}$ and $P_{b,j+1}$ as the coarse-scale pressures, respectively. The distance between the centers of the two columns is $\Delta Z = Z_{j+1} - Z_j$. $u_{\text{tot},j+1/2}$ is the total flux from layer $j$ to layer $j+1$, through boundary $\zeta_{j+1}$.

Eqs. (5.6) and (5.7) give a complete coarse-scale pressure equation for a single layer system. However, for a multilayer system, the layers are coupled and $u_{\text{tot},z}|_{\zeta_T}$ and $u_{\text{tot},z}|_{\zeta_B}$ are non-zero. We need to derive a coarse-scale equation for $u_{\text{tot},z}|_{\zeta_T}$ and $u_{\text{tot},z}|_{\zeta_B}$ that couples the neighbor layers. Without loss of generality, we take the flux between layer $j$ and layer $j+1$ as an example (see Figure 5.2). Note that we choose the flux between layer $j$ and layer $j+1$ as the primary variable for pressure. We approximate the total flux between the two layers as

$$u_{\text{tot},j+1/2} = -K_{z,j+1/2}\Lambda_{\text{tot},j+1/2}\left(\frac{P_{b,j+1} - P_{b,j}}{\Delta Z} + \Omega_{1,j+1/2} + \Omega_{2,j+1/2}\right),$$  

(5.8)

where $K_{z,j+1/2}$ and $\Lambda_{\text{tot},j+1/2}$ are the effective coarse-scale permeability and total mobility, respectively, between the two layers; $\Omega_{1,j+1/2}$ and $\Omega_{2,j+1/2}$ are terms associated with capillary pressure and gravity respectively; $\Delta Z = Z_{j+1} - Z_j$ with $Z_j$ and $Z_{j+1}$ the $z$ values of the centers of layer $j$ and $j+1$, respectively; $P_{b,j}$ and $P_{b,j+1}$ are the coarse-scale brine pressures defined as the brine pressure at $Z = Z_j$ and $Z = Z_{j+1}$, respectively.
The coefficients $K_{c,j+1/2}$, $\Lambda_{\text{tot},j+1/2}$, $\Omega_{1,j+1/2}$ and $\Omega_{2,j+1/2}$ are defined based on the fine-scale equations for the two fluid phase fluxes in the vertical direction, which can be written as

$$u_{b,z} = -k_z \lambda_b \left( \frac{\partial p_b}{\partial z} + \rho_b g \right),$$  \hspace{1cm} (5.9a)

$$u_{c,z} = -k_z \lambda_c \left( \frac{\partial p_c}{\partial z} + \rho_c g \right).$$  \hspace{1cm} (5.9b)

Summing Equation (5.9a) and (5.9b), and we obtain the equation for total flux

$$u_{\text{tot},z} = -k_z (\lambda_b + \lambda_c) \frac{\partial p_b}{\partial z} - k_z \lambda_c \frac{\partial p_c^{\text{cap}}}{\partial z} - k_z (\lambda_b \rho_b + \lambda_c \rho_c) g.$$  \hspace{1cm} (5.10)

Rearranging Equation (5.10) gives

$$\frac{\partial p_b}{\partial z} = -\frac{u_{\text{tot},z}}{k(\lambda_b + \lambda_c)} - \frac{\lambda_c}{\lambda_b + \lambda_c} \frac{\partial p_c^{\text{cap}}}{\partial z} - \frac{(\lambda_b \rho_b + \lambda_c \rho_c)}{\lambda_b + \lambda_c} g.$$  \hspace{1cm} (5.11)

Integrating Equation (5.11) from $Z_j$ to $Z_{j+1}$ with respect to $z$ yields

$$\int_{Z_j}^{Z_{j+1}} \frac{\partial p_b}{\partial z} \, dz = -\int_{Z_j}^{Z_{j+1}} \frac{u_{\text{tot},z}}{k(\lambda_b + \lambda_c)} \, dz - \int_{Z_j}^{Z_{j+1}} \frac{\lambda_c}{\lambda_b + \lambda_c} \frac{\partial p_c^{\text{cap}}}{\partial z} \, dz - \int_{Z_j}^{Z_{j+1}} \frac{(\lambda_b \rho_b + \lambda_c \rho_c)}{\lambda_b + \lambda_c} g \, dz.$$  \hspace{1cm} (5.12)

The left-side term can be written as

$$\int_{Z_j}^{Z_{j+1}} \frac{\partial p_b}{\partial z} \, dz = P_{b,j+1} - P_{b,j},$$  \hspace{1cm} (5.13)

To derive the coefficients in Equation (5.8), we take $u_{\text{tot},Z_{j+1/2}}$ as an approximation for the average total flux from $Z_j$ to $Z_{j+1}$ in $z$ direction and obtain

$$\int_{Z_j}^{Z_{j+1}} \frac{u_{\text{tot},z}}{k_z (\lambda_b + \lambda_c)} \, dz \approx u_{\text{tot},Z_{j+1/2}} \int_{Z_j}^{Z_{j+1}} \frac{1}{k_z (\lambda_b + \lambda_c)} \, dz.$$  \hspace{1cm} (5.14)
Substituting Equation (5.13) and (5.14) into Equation (5.12) and after some rearrangement, we obtain

\[
u_{\text{tot},Z_{j+1/2}} = -\frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \frac{1}{k_c(\lambda_b + \lambda_c)} \left[ \frac{P_{b,j+1} - P_{b,j}}{\Delta Z} + \frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \frac{\lambda_c}{\lambda_b + \lambda_c} \frac{\partial p^{cap}}{\partial z} \, dz + \frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \left( \frac{\lambda_b \rho_b + \lambda_c \rho_c}{\lambda_b + \lambda_c} \cdot \gamma \right) \, dz \right]. \tag{5.15}
\]

Comparing to Equation (5.8), we obtain

\[
K_{z,j+1/2}A_{\text{tot},j+1/2} = -\frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \frac{1}{k_c(\lambda_b + \lambda_c)} \, dz, \tag{5.16a}
\]

\[
\Omega_{1,j+1/2} = \frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \frac{\lambda_c}{\lambda_b + \lambda_c} \frac{\partial p^{cap}}{\partial z} \, dz, \tag{5.16b}
\]

\[
\Omega_{2,j+1/2} = \frac{1}{\Delta Z} \int_{Z_j}^{Z_{j+1}} \left( \frac{\lambda_b \rho_b + \lambda_c \rho_c}{\lambda_b + \lambda_c} \cdot \gamma \right) \, dz. \tag{5.16c}
\]

Note that the derived coarse-scale vertical transmissivity \(K_{z,j+1/2}A_{\text{tot},j+1/2}\) between layer \(j\) and \(j+1\) is a harmonic average of the fine-scale vertical transmissivities, which is consistent with the classic average scheme of vertical hydraulic conductivities.

Similarly, we can obtain the flux between layer \(j-1\) and \(j\), \(\nu_{\text{tot},Z_{j-1/2}}\). Then, substituting the two fluxes \(\nu_{\text{tot},Z_{j-1/2}}\) and \(\nu_{\text{tot},Z_{j+1/2}}\) into Equation (5.6), we obtain the coarse-scale pressure equation that couples the neighbor layers \(j-1\), \(j\) and \(j+1\)

\[
(c_p H_j + c_b \Phi_j S_{b,j} + c_c \Phi_j S_{c,j}) \frac{\partial P_{b,j}}{\partial t} + (c_p H_j + c_c \Phi_j) S_{c,j} \frac{\partial p^{cap}}{\partial t} + \nabla \cdot \left( -K_{\|,j}(\lambda_b \nabla \| \pi_j + \lambda_c \nabla \| \pi_j \nabla p^{cap} \right)
\]

\[
= -K_{z,j+1/2}A_{\text{tot},j+1/2} \left( \frac{P_{b,j+1} - P_{b,j}}{\Delta Z} + \Omega_{1,j+1/2} + \Omega_{2,j+1/2} \right)
+ K_{z,j-1/2}A_{\text{tot},j-1/2} \left( \frac{P_{b,j} - P_{b,j-1}}{\Delta Z} + \Omega_{1,j-1/2} + \Omega_{2,j-1/2} \right) \tag{5.17}
+ \Psi_j^b + \Psi_j^c.
\]
5.3.3 Fine-scale transport in each layer

On the fine scale within each individual layer, we use a dynamic reconstruction algorithm similar to the one developed in Guo et al. (2014a). Here, we only outline the main steps of the algorithm; for further details, please see Guo et al. (2014a).

We need to reconstruct both the saturation and pressure on the fine scale. We reconstruct the fine-scale pressure using a saturation weighted hydrostatic pressure profile with the pressure at the center of the layer (along $z$ axis) fixed as the updated coarse-scale pressure. Other choices for pressure reconstruction have been discussed in Guo et al. (2014a,b), and the results to date indicate that the saturation weighted hydrostatic reconstruction gives the best results. The reconstructed fine-scale pressure field is then used to compute the horizontal fine-scale phase fluxes. The total fluxes from the bottom and the top of each layer are computed from Equation (5.8) in the coarse-scale calculation. Then, the horizontal fluxes between the columns and the fluxes at the top and bottom of columns are all computed, and we only need to solve the vertical columns (see Figure 5.1) as independent one-dimensional problems. These one-dimensional problems have “counter-current” type of flow involving buoyancy-driven upward migration of CO$_2$ and gravity-driven downward drainage of brine, which we solve with a fractional flow formulation as shown in Equation (5.18a) and (5.18b). Note that the total fluxes $u_{\text{tot},z}$ are nonzero; they are computed from the fine-scale horizontal total fluxes and the total fluxes at the top and the bottom of the layer. From the fine-scale phase fluxes computed from the fractional flow equations, we then compute and reconstruct the CO$_2$ saturation in each column.

\begin{align}
    u_{b,z} &= f_b \left( u_{\text{tot},z} - k_z \lambda_c \Delta \rho g + \lambda_c k_z \frac{\partial \rho_{\text{cap}}}{\partial z} \right) \quad (5.18a) \\
    u_{c,z} &= f_c \left( u_{\text{tot},z} + k_z \lambda_b \Delta \rho g - \lambda_b k_z \frac{\partial \rho_{\text{cap}}}{\partial z} \right) \quad (5.18b)
\end{align}
5.3.4 Numerical scheme

The set of multiscale equations in sections 5.3.2 and 5.3.3 are solved numerically. We use an IMPES (implicit pressure explicit saturation) type method for time stepping and a finite volume method for spatial discretization. The (coarse-scale) pressure is solved implicitly and the (fine-scale) transport is solved explicitly. The two scales are coupled sequentially (see Figure 5.1). See Appendix 5.A for details of the numerical discretization.

5.4 Model comparison

The multilayer dynamic reconstruction model (from this point forward, we refer to it as MLDR) developed in this chapter can simulate CO$_2$ migration in a layered heterogeneous formation. To show the capability of the MLDR model, we compare it with the widely used full three-dimensional multiphase flow simulator TOUGH2/ECO2N developed at Lawrence Berkeley National Lab (Pruess et al., 1999; Pruess, 2005). For the comparison, we use two kinds of test cases. The first one has a simple two-layer geologic formation with idealized parameter sets, while the other has a four-layer geologic formation with parameters from the Mt Simon formation of the Illinois Basin. For the first test case with two-layers, we assign different permeabilities to the two layers. Three different scenarios are tested, all of which have a lower permeable layer sitting above a higher permeable layer, but with different permeability contrasts (see Table 5.1). For the Mt Simon inspired test case, the parameter sets are given in Table 5.2, and are based on the data from Zhou et al. (2010).

5.4.1 A simple two-layer geologic formation

For the two-layer scenarios, the two layers are both homogeneous and isotropic, and, except for different permeabilities, all other parameters are kept the same for the three scenarios. The pairs of permeabilities for the two layers are (10 mD, 100 mD), (1 mD, 100 mD) and
Porosity is 0.25 and the system is isothermal with a temperature fixed at 35 °C. Density and viscosity of the two fluid phases are fixed as constants in the MLDR model, while TOUGH2 has an equation of state to compute fluid properties from temperature and pressure. The CO₂ injection rate is 1.0 Mt/year (= 10⁹ kg/year), and CO₂ is injected from a vertical well over the entire thickness of the bottom layer. A boundary condition of hydrostatic pressures are used in the far field of the domain and the formation is initially saturated with brine. Taking advantage of the symmetry of the domain, we choose a quarter domain with an injection rate of 0.25 Mt/year to run the models.

The residual saturations of CO₂ and brine is \( s_{b,r} = 0.3 \) and \( s_{c,r} = 0 \), respectively. We use the van Genuchten model to parameterize relative permeability and capillary pressure, with the characteristic capillary pressure \( \alpha^{-1} = 10 \text{ Pa} \) and the pore-size distribution coefficient \( m = 0.99 \). The entire formation has a thickness of 50m and each layer is 25 m thick. The top of the formation has a depth of 1000m. The horizontal extent of the quarter domain is 5 km in both x and y directions. The numerical resolution in the vertical is uniform with \( \Delta z = 1 \text{ m} \) and the grid size in the horizontal progressively increases from \( \Delta x = \Delta y = 5 \text{ m} \) close to the injection well to \( \Delta x = \Delta y = 100 \text{ m} \) at the boundary. The number of numerical grid cells is 120 in both x and y directions.

The simulation times for the three scenarios are all 5 years and comparisons are made at 1 and 5 years, respectively. Results from the MLDR model show good agreement with those from TOUGH2 for all the three scenarios, as can be seen in Figures 5.3 - 5.5. We measure the difference with two metrics: the mass of CO₂ in each layer and extent of the CO₂ plume at the top of each layer. As shown in Table 5.1, the CO₂ mass distribution from the two models in the two layers is very close; the difference between the models is always less than 2% when normalized by the amount injected, with most cases well less than 1%. The extent of the plumes is also in very good agreement. The differences are within 1 to 3 numerical grid cells. In terms of computational time, it took 14.6 hours, 12.0 hours and 63.7 hours for the MLDR model to finish the three scenarios, respectively, on a 2011 iMac.
<table>
<thead>
<tr>
<th>permeability $k$ (mD)</th>
<th>model</th>
<th>$t = 1$ year</th>
<th></th>
<th>$t = 5$ years</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>upper layer</td>
<td>lower layer</td>
<td>upper layer</td>
<td>lower layer</td>
</tr>
<tr>
<td>$k_{upper} = 10$, $k_{lower} = 100$</td>
<td>MLDR</td>
<td>19.30</td>
<td>45</td>
<td>80.70</td>
<td>575</td>
</tr>
<tr>
<td></td>
<td>TOUGH2</td>
<td>18.70</td>
<td>60</td>
<td>81.30</td>
<td>550</td>
</tr>
<tr>
<td></td>
<td>difference</td>
<td>0.60</td>
<td>15</td>
<td>0.60</td>
<td>25</td>
</tr>
<tr>
<td>$k_{upper} = 1$, $k_{lower} = 100$</td>
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<td>-</td>
<td>95.15</td>
<td>675</td>
</tr>
<tr>
<td></td>
<td>TOUGH2</td>
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<td>-</td>
<td>95.41</td>
<td>700</td>
</tr>
<tr>
<td></td>
<td>difference</td>
<td>0.26</td>
<td>-</td>
<td>0.26</td>
<td>25</td>
</tr>
<tr>
<td>$k_{upper} = 10$, $k_{lower} = 1000$</td>
<td>MLDR</td>
<td>28.30</td>
<td>-</td>
<td>71.70</td>
<td>700</td>
</tr>
<tr>
<td></td>
<td>TOUGH2</td>
<td>28.71</td>
<td>-</td>
<td>71.29</td>
<td>725</td>
</tr>
<tr>
<td></td>
<td>difference</td>
<td>0.41</td>
<td>-</td>
<td>0.41</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 5.1: Comparisons of MLDR model and TOUGH2 for a two-layer formation. $M$ is the mass of CO$_2$ in each layer normalized by the amount injected, $R_1$ and $R_2$ are the extent of the CO$_2$ plume at the top of layer 1 and layer 2, respectively, as shown in Figure 5.3 for example. '-' indicates that CO$_2$ has not reached the top of the layer.

using a single intel i7 processor. The corresponding computational times are 43 hours, 35 hours and 78.5 hours for TOUGH2 on a cluster with 20 processors. Thus, the MLDR model with our implementation is roughly 20 to 60 times more efficient than TOUGH2 for the scenarios we considered.

### 5.4.2 A Multi-layer geologic formation

To further demonstrate the practical applicability of the MLDR model, we choose a more realistic geologic formation with multiple layers. The formation we consider has four layers, and each of them has different geologic properties. The geologic parameters for the layers (see Table 5.2) are representative values chosen from the Mt Simon formation of the Illinois Basin as reported in Zhou et al. (2010). We use the same capillary pressure and relative permeability curves from the first test case in section 5.4.1 for all the four layers. The total thickness of the formation is 60 m and the depth at the top is 2400 m. The size of the domain in the horizontal, the resolution of the numerical grid and the number of grid cells are kept the same as for the first test case.
Figure 5.3: CO$_2$ plume comparison between the MLDR model and TOUGH2 for a two-layer formation with permeability of 10 mD and 100 mD in the upper and lower layers, respectively. The first row shows the CO$_2$ plume from the MLDR model and the second row shows that from TOUGH2. The plumes in the left column are after 1 year of injection and those in the right column are after 5 years of injection. The CO$_2$ plume extent at the top of each layer is marked in the right-top corner panel as an example. Note that the plumes we show here are vertical cross-sections of a three-dimensional domain that passes through the injection well, and this applies to Figures 5.4–5.6 as well.

Figure 5.4: CO$_2$ plume comparison between the MLDR model and TOUGH2 for a two-layer formation with permeability of 1 mD and 100 mD in the upper and lower layers, respectively. The first row shows the CO$_2$ plume from the MLDR model and the second row shows that from TOUGH2. The plumes in the left column are after 1 year of injection and those in the right column are after 5 years of injection.
Figure 5.5: CO₂ plume comparison between the MLDR model and TOUGH2 for a two-layer formation with permeability of 10 mD and 1000 mD in the upper and lower layers, respectively. The first row shows the CO₂ plume from the MLDR model and the second row shows that from TOUGH2. The plumes in the left column are after 1 year of injection and those in the right column are after 5 years of injection.

Again, the CO₂ plumes from the two models are almost indistinguishable (see Figure 5.6). We computed the mass of CO₂ and the extent of the CO₂ plume at the top of each individual layer from both simulators. The difference is very small (see Table 5.3), as is expected from the good visual agreement of the CO₂ plumes in Figure 5.6. The maximum difference of CO₂ mass is less than 1% of the total mass injected, and the difference of the CO₂ plume extent is all within one grid cell. In terms of computational time, the MLDR simulator used about 50 hours on a 2011 iMac using a single intel i7 processor, while it took more than 200 hours for TOUGH2 to finish the simulation on a cluster with 10 processors. Thus, the MLDR model with our implementation is roughly 40 times more efficient than TOUGH2 for the four-layer test case we considered.

Finally, we note that the implementation of the MLDR model assumes constant density and viscosity of the two fluids. The density we used in the simulation shown herein is the saturation weighted density from results of the TOUGH2 simulations, and the viscosity is computed from the pressure corresponding to the computed saturation weighted density. Despite the assumption of constant density and viscosity in the MLDR model, the
predictions of CO₂ plumes are in very good agreement with those from TOUGH2. This is because the density and viscosity do not have much variation in the test cases we considered and therefore it is reasonable to assume constant density and viscosity. In fact, a simple estimation of density and viscosity from the initial pressure in the formation (before CO₂ is injected) is very close to what we got from the TOUGH2 simulation. Nevertheless, for geologic formations where variations in density and viscosity are important, an equation of state needs to be implemented for each of the fluid phases in the MLDR model.

### 5.5 Discussion

The MLDR model captures the vertical dynamics of CO₂ and brine well both within each individual layer and between the layers. All comparisons of MLDR and TOUGH2 show excellent results. Further, the MLDR algorithm significantly reduces computational effort
<table>
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<th>thickness</th>
<th>$\phi$</th>
<th>$k_h$</th>
<th>$k_v$</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>(m)</td>
<td>-</td>
<td>(mD)</td>
<td>(mD)</td>
</tr>
<tr>
<td>1</td>
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<tr>
<td>2</td>
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</tr>
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<td>5.1</td>
</tr>
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<td>4</td>
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<td>0.18</td>
<td>891.5</td>
<td>731.5</td>
</tr>
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</table>

Table 5.2: Geologic parameters of a four-layer formation

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<th>model</th>
<th>t = 1 year</th>
<th>t = 5 years</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>M (%)</td>
<td>R (m)</td>
</tr>
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<td>MLDR</td>
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<td>80</td>
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<tr>
<td></td>
<td>TOUGH2</td>
<td>0.22</td>
<td>80</td>
</tr>
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<td>difference</td>
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<td>difference</td>
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<td></td>
<td>difference</td>
<td>0.13</td>
<td>0</td>
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</table>

Table 5.3: Comparisons of MLDR model and TOUGH2 for a four-layer formation. $M$ is the mass of CO$_2$ in each layer normalized by the amount injected, $R$ is the extent of the CO$_2$ plume at the top of each layer.
compared to full three-dimensional models. In the MLDR model, pressures are only solved on the coarse scale. The size of the matrix to solve the pressure equation is significantly reduced compared to a full three-dimensional model, where all the fine-scale pressures needed to be solved. Also, the remaining fine-scale one-dimensional “counter-current” flow problem is easy to solve using the fractional flow formulation. Thus, the multilayer dynamic reconstruction algorithm leads to significant reduction of computational effort. Here, we take a geologic formation with three layers as an example and give a simple analysis of the complexity of the algorithm. The pressure solver of the MLDR model has a complexity of \(O(N_x^2 \times N_y^2 \times 3^2)\), while the full three-dimensional model has a complexity of \(O(N_x^2 \times N_y^2 \times (N_{z1} + N_{z2} + N_{z3})^2)\). \(N_x\) and \(N_y\) are the number of grid cells in \(x\) and \(y\) directions, respectively. \(N_{z1}\), \(N_{z2}\) and \(N_{z3}\) are the numbers of vertical grid cells in each of the three layers. This simple analysis shows that the MLDR algorithm reduces the computational cost by an order of \(O((N_{z}/3)^2)\), where \(N_z = N_{z1} + N_{z2} + N_{z3}\) is the total number of numerical grids in \(z\) direction. It should be noted that the pressure solution is the most computationally intensive part of both the MLDR and conventional three-dimensional algorithms. Although, we recognize that TOUGH2 may be slowed partially by the additional computation of component transport and inclusion of compressibility, for the simulations presented here, despite that the implementation of the MLDR is not much optimized, the MLDR model is at least 20 times more computationally efficient compared to TOUGH2; it is 40 to 60 times faster for most of the simulations we have analyzed.

We note because the MLDR model uses an explicit scheme for the fine-scale one-dimensional problem, it may require small time steps when the \(\text{CO}_2\) and brine segregate rapidly in the vertical. Nevertheless, in the simulations we have done, the smallest time step does not appear to be unreasonably small. Furthermore, when the time step becomes restrictive, several remediation strategies are available. Here, we propose three of them. First, we can use larger time steps for the coarse scale than for the fine scale, that is, we compute for several time steps on the fine scale within one coarse-scale time step with a
constrain of mass balance. In addition, those fine-scale one-dimensional problems can be computed in parallel because they are independently solved in the MLDR multiscale framework. Finally, if the time step becomes small due to rapid fluid segregation, it is likely that CO$_2$ and brine reach vertical equilibrium quickly in some of the layers. Thus, it is natural to directly use the (analytical) VE reconstruction without any time step restriction for those layers instead of the dynamic reconstruction algorithm.

For a layered geologic formation with significant contrast in permeabilities between the layers, as mentioned in the previous paragraph, VE reconstruction can be used for layers with high permeability where buoyant segregation is fast and the flow is essentially horizontal; while layers with very low permeability may be treated as “aquitard”, and we just model the vertical flow, neglecting the horizontal flow, following the tangent law, see e.g. (Bear, 1972; Nordbotten and Celia, 2012). Such multilayer systems with alternating “aquifers” and “aquitards” have been studied in groundwater hydrology (e.g., Hunt, 1985; Hemker and Maas, 1987) and later in the context of CO$_2$ sequestration for CO$_2$ migration and leakage through abandoned wells (e.g., Nordbotten et al., 2004, 2009; Cihan et al., 2011; Bandilla et al., 2012). We note that all of these multilayer models either only focus on single phase flow or use VE reconstructions for a two-phase flow system. Our MLDR model extends this alternating “aquifer-aquitard” system to a general multilayer model that can include vertical two-phase flow dynamics in layers when VE reconstruction is inappropriate and when flow in low-permeability (“aquitard”) formations is not only in the vertical. This extension leads to a new class of hybrid multilayer models where we can design the reconstruction of each layer based on the dominant physics in that layer: use VE or DR reconstructions in the vertical direction depending on the time scales of buoyant segregation of the two fluid phases in aquifers, as well as possible simplified “aquitard” models for the vertical direction when horizontal flow is negligible. For layers with significant heterogeneity with weak horizontal correlation, we can use a full three-dimensional model for that particular layer and still use vertically-integrated models with reconstruction algo-
gorithms or “aquitard” models for other layers, thereby maintaining computational efficiency. Overall, the MLDR algorithm offers a framework to further develop more advanced hybrid models for CO₂ migration in layered geologic formations.

Finally, we point out the similarities and differences for the multiscale multilayer algorithm compared to two existing numerical methods: the Alternating Direction Implicit (ADI) method and the Multiscale Finite Volume Method (MsFVM). The ADI method, developed in the 1950s (Peaceman and Rachford, 1955; Douglas and Rachford, 1956), is a numerical method that reduces the multi-dimensional problems into repeated one-dimensional problems with tridiagonal matrices that can be effectively solved using the Thomas algorithm. Subsequent developments of ADI-like methods involved three-dimensional problems solved as a combination of two-dimensional (horizontal) solutions and one-dimensional (vertical) solutions (Babu and Pinder, 1984). This type of alternating-direction method is similar to the single layer DR algorithm (Guo et al., 2014a) in that two-dimensional horizontal solutions are coupled with one-dimensional vertical solutions. However, the fundamental difference between the single layer DR algorithm and the ADI is that the single layer DR only solves one horizontal plane obtained from vertical integration, as opposed to the ADI method that solves many horizontal planes (with the number equals to the number of vertical grid cells). The MLDR algorithm, an extension to the DR, differs even more from the ADI method. The MLDR coarse scale is a three-dimensional problem - it solves the horizontal flow within each layer and vertical flow between the layers. This kind of two-scale resolution does not exist in the classical ADI methods.

The other numerical method we want to compare is the MsFVM, which is a numerical method that, based on finite-volume descretization, solves the pressure equation on a coarse scale and the transport equation on a fine scale, (see e.g. Jenny et al., 2003, 2005). The MLDR algorithm can be cast into the framework of MsFVM if we think of the coarse-scale cell of the MLDR algorithm as a coarse-scale cell in the MsFVM with 1 x 1 x N fine-scale
cells in \( x, y \) and \( z \) directions, respectively. The MsFVM computes coarse-scale effective transmissivities using pressure basis functions, and constructs a coarse-scale system for the pressure equation with the coarse-scale effective transmissivities, then it projects the coarse-scale solutions onto the fine grid by applying the basis functions. The MLDR algorithm, however, only uses the multiscale idea for the vertical dimension. Instead of using specialized basis functions as in MsFVM, the effective transmissivities in MLDR are derived from vertical integration. Thus, although MLDR can be cast into the general MsFVM framework, it is a novel multiscale algorithm developed by using vertical integration and reconstruction operators.

5.6 Conclusion

In this chapter, we present a multilayer dynamic reconstruction algorithm that can simulate \( \text{CO}_2 \) migration in deep saline aquifers with layered heterogeneity. The algorithm is based on casting the full three-dimensional governing equations into two scales. The coarse scale is the multiple vertically integrated layers, with coarse-scale pressure only a function of \((x,y)\) in any layer, and a coarse-scale pressure equation that couples all the layers. The fine scale corresponds to the vertical one-dimensional columns defined within the thickness of each layer, on which we solve the two-phase flow dynamics of \( \text{CO}_2 \) and brine with the dynamic reconstruction algorithm from \cite{Guo2014}. Results show that the MLDR model is in excellent agreement with a full three-dimensional simulator (TOUGH2) for all the test cases we considered. The MLDR model is also much more computationally efficient compared to TOUGH2, with computational time 20 to 60 times smaller for MLDR.

In summary, the MLDR model is accurate and much more computationally efficient than conventional full three-dimensional simulators, and the computational advantages make it an attractive tool for simulations of \( \text{CO}_2 \) migration in large-scale \( \text{CO}_2 \) sequestration systems. In addition, the MLDR model provides a modeling framework for \( \text{CO}_2 \) migration...
in geologic formation with layered heterogeneities, which can lead to the development of a new class of hybrid models where different reconstructions can be chosen for different layers based on their different time scales of buoyant segregation.

5.A Appendix: Numerical scheme

A time stepping scheme analogous to the implicit pressure - explicit saturation (IMPES) method is used in this chapter. We solve pressure on the coarse scale (multiple vertically-integrated layers) implicitly, while solve the saturation on the fine scale explicitly. Equation (5.19) shows the time discretization of the coarse-scale pressure equation. We linearize the equation by lagging one time step for the coefficients, e.g. mobilities and capillary pressure.

\[
(c_b \Phi_j S^n_{b,j} + c_c \Phi_j S^n_{c,j}) \frac{P^{n+1}_{b,j} - P^n_{b,j}}{\Delta t} + (c_b H_j + c_c \Phi_j) S^n_{c,j} \frac{P^{cap,n} - P^{cap,n-1} j}{\Delta t}
\]

\[
+ \nabla \cdot \left( -K_{\parallel,j} (\lambda_{b,j} + \lambda_{c,j}) \nabla P^n_{b,j} - K_{\parallel,j} (\rho_b \lambda_{b,j} + \rho_c \lambda_{c,j}) G_j - K_{\parallel,j} \lambda_{c,j} \nabla P^{cap,n} j \right)
\]

\[
= -K_{c,j+1/2} \Lambda^n_{tot,j+1/2} \left( \frac{P^{n+1}_{b,j} - P^n_{b,j}}{\Delta Z} + \Omega^n_{1,j+1/2} + \Omega^n_{2,j+1/2} \right)
\]

\[
+ K_{c,j-1/2} \Lambda^n_{tot,j-1/2} \left( \frac{P^{n+1}_{b,j} - P^n_{b,j-1}}{\Delta Z} + \Omega^n_{1,j-1/2} + \Omega^n_{2,j-1/2} \right) + \Psi^{b,n+1} j + \Psi^{c,n+1} j
\]

From equation (5.19), we can compute the coarse-scale pressure field. Once we obtain the coarse-scale pressure field, the rest of the numerical solution procedure is similar to the dynamic reconstruction in a single layer case, and we can directly follow the section 3.3 in Guo et al. (2014a) to reconstruct the fine-scale saturation and pressure.
Chapter 6

Model Extensions

The multiscale algorithms presented in Chapters 4 and 5 can be extended to develop some advanced models that are applicable to CO$_2$ sequestration in more complex geologic systems and some other energy and environmental problems. This chapter introduces two directions of extensions: one towards the development of hybrid models, and the other towards the development of vertically-integrated models for CO$_2$ sequestration in fractured reservoirs.

6.1 Hybrid models

6.1.1 Hybrid multi-layer vertically-integrated models

As briefly discussed in Chapter 5, we can combine the different model options to form a hybrid multi-layer vertically-integrated model. The geologic layers of a multi-layer geologic formation can be categorized into four types: homogeneous (or mild heterogeneous layers that can be assumed to be homogeneous) layers with low permeability, intermediate permeability, and high permeability, and layers with strong heterogeneity. Modeling options are available for each type of layers: 1) The low permeability homogeneous layers, when they are part of a stratigraphic column of alternating high- and low-permeability
layers, can be assumed to have essentially vertical flows between the top and bottom high-permeability layers. This can be modeled by a simple vertical one-dimensional “aquitard” model; 2) In the high permeability homogeneous layers, CO$_2$ and brine segregate quickly, and the vertical equilibrium model can be applied; 3) For the intermediate permeability homogeneous layers, we use the dynamic reconstruction algorithm from Chapter 4; 4) For the layers with strong multi-dimensional heterogeneity, with heterogeneity in both horizontal and vertical directions, vertically-integrated models usually do not apply and full three-dimensional models need to be used. Finally, for the sequence of layers, the multi-layer coupling algorithm developed in Chapter 5 can be used to couple the different layers.

Successful development of a multi-layer hybrid model relies on a robust criterion to categorize the different types of layers. The vertical equilibrium layers can be identified by estimating the time scale for the vertical buoyant segregation, where the vertical equilibrium model applies when the time scale is small relative to the overall simulation time. The low permeability layers can be defined using the tangent law, which suggests that a low permeability layer sitting below and above high permeability layers will have essentially vertical flow as long as their permeability ratio $k_{\text{low}}/k_{\text{high}} \leq 0.1$ (Bear, 1972; Pinder and Celia, 2006). Thus, we can define the low permeability layers based on the permeability contrast from their neighbor layers.

The hybrid multi-layer model allows use of a combination of models with different levels of complexity, as opposed to using the computationally demanding full three-dimensional models for the entire formation. With a carefully considered model-switching criterion, the hybrid multi-layer model can serve as a powerful computational tool for simulation studies of the multiphase flows for CO$_2$ injection and migration in layered geological formations.
6.1.2 Hybrid multi-dimensional models

Another hybrid extension is a hybrid multi-dimensional model, the idea of which is to use different models for different sub-domains in the horizontal direction. The three-dimensional models can be used for the sub-domains in which heterogeneities are important, e.g. the sub-domain in the vicinity of the injection wells and leakage pathways. For the sub-domains where small scale heterogeneity does not play a significant role, we can use either the vertical equilibrium model or the dynamic reconstruction models, depending on whether the vertical equilibrium assumption is invalid. The different sub-domains are coupled at the interfaces with monolithic coupling schemes, which solve the sub-domains simultaneously.

The development of the hybrid multi-dimensional models is an ongoing collaborative project with Prof. Rainer Helmig’s group at the University of Stuttgart, which is part of a large effort to develop modeling tools to investigate the potential of geological storage of hydrogen and methane as energy storage options for the intermittent renewable energy resources (mainly solar and wind) in Germany.

6.2 Vertically-integrated models for CO$_2$ injection in fractured reservoirs

Compared to a conventional unfractured reservoir, a fractured reservoir consists of porous rock blocks as well as fractures through which fluids can flow readily. The fractures have large permeability but provide little overall porosity, while the rock blocks (often referred to as matrix) are much less permeable than the fractures, but they provide most of the pore spaces. Due to the permeability contrast between the fractures and the matrix, the flow in the fracture is much faster than that in the matrix, leading to two different characteristic time scales.
This section reviews some of the mathematical models that have been developed for multiphase flow in fractured reservoirs, and presents a new vertically-integrated dual-porosity dual-permeability model for CO$_2$ injection and migration in fractured geologic formations.

6.2.1 Background: three-dimensional dual-porosity dual-permeability models

At the reservoir scale, the fracture flow models often treat the fractures as a continuum, as it is generally computationally infeasible to resolve every individual fracture. The early work of [Barenblatt et al., 1960] and [Warren and Root, 1963] both considered the fractures as a continuum. [Barenblatt et al., 1960] developed a so-called dual-permeability model, where the matrix was treated as another continuum with a different permeability and porosity, and the flow in the matrix was considered. [Warren and Root, 1963] developed a so-called dual-porosity model, where the authors approximated the rock blocks (matrix) as equal-sized cubes with homogeneous and isotropic rock properties that are not connected to one another except through the fractures. The fluid pressure in the matrix blocks is uniform, and fluid in the matrix only exchanges with fluid in the fractures. For both the dual-permeability and dual-porosity models, the transfer of mass between fractures and matrix is the key process, which is often represented by a mass transfer function. In principle, the mass transfer function needs to include the shape of the matrix blocks and the various forces that drive the mass exchanges, such as capillary pressure, gravity and viscous forces. Some more advanced work accounts for non-uniform pressure and saturation distributions within the blocks, and allows advective flows in the matrix blocks. Many improvements have been made after the pioneer work of [Barenblatt et al., 1960] and [Warren and Root, 1963], especially in the development of the mass transfer functions. Recent reviews of various versions of the mass transfer functions can be found in [Ramirez et al., 2009] and [Al-Kobaisi et al., 2009].
Both the dual-porosity model and the dual-permeability model consider the fractures as a continuum, where the Darcy’s Law applies for the fluid flow dynamics. For a homogeneous and isotropic fracture domain, we define $\phi^f$ and $k^f$ as the porosity and permeability (assuming isotropic permeability), respectively, $s^f_\alpha$ the phase saturation, $\rho^f_\alpha$ the density of the fluid, and $p^f_\alpha$ the phase pressure. The superscript $f$ denotes that the parameters are defined in the fracture domain, and the subscript $\alpha = c$ or $b$ represents CO$_2$ ($\alpha = c$) or brine ($\alpha = b$). Assuming that CO$_2$ and brine are immiscible and incompressible, we can write mass balance equations for both the CO$_2$ and brine phases

$$\frac{\partial (\phi^f s^f_\alpha)}{\partial t} + \nabla \cdot \mathbf{u}^f = q^{m-f}_\alpha + \psi^f_\alpha,$$  \hspace{1cm} (6.1)

$$\frac{\partial (\phi^f s^f_\alpha)}{\partial t} + \nabla \cdot \mathbf{u}^f = q^{m-f}_\alpha + \psi^f_\alpha,$$  \hspace{1cm} (6.2)

where $q^{m-f}_c$ and $q^{m-f}_b$ represent CO$_2$ and brine volumetric fluxes from the matrix to the fracture domain, respectively; $\psi^f_c$ and $\psi^f_b$ denote the volumetric source terms of CO$_2$ and brine in the fractures, respectively; and the CO$_2$ and brine phase fluxes $\mathbf{u}^f_c$ and $\mathbf{u}^f_b$ can be obtained from the two-phase Darcy’s Law

$$\mathbf{u}^f_c = -\frac{k^{f,c}}{\mu_c} (\nabla p^f_c - \rho_c \mathbf{g}),$$  \hspace{1cm} (6.3)

$$\mathbf{u}^f_b = -\frac{k^{f,b}}{\mu_b} (\nabla p^f_b - \rho_b \mathbf{g}).$$  \hspace{1cm} (6.4)

The difference between the dual-porosity and the dual-permeability models lies in the flow model for the matrix. The dual-porosity represents the matrix as an immobile domain that only exchanges fluid with the fractures and provides volumes for storage. The dual-permeability model represents the matrix as a continuum domain that fluids can flow
through. We present the governing equations for the matrix in both the dual-porosity and dual-permeability models, and also for the matrix in a modified dual-permeability model.

**Dual-porosity model**

In the dual-porosity model, the fluids in the matrix are assumed immobile and only exchange mass with the fracture domain. Thus, we obtain the following governing equations for the matrix

\[
\frac{\partial (\phi^m s^m c)}{\partial t} = q^f_{c^m} + \psi^m_c,
\]

(6.5)

\[
\frac{\partial (\phi^m s^m b)}{\partial t} = q^f_{b^m} + \psi^m_b,
\]

(6.6)

where superscript \( m \) represents matrix, and \( q^f_{c^m} \) and \( q^f_{b^m} \) denote the CO\(_2\) and brine volumetric fluxes from the fracture domain to the matrix domain, respectively; \( \psi^m_c \) and \( \psi^m_b \) are the volumetric source terms of CO\(_2\) and brine in the matrix.

**Dual-permeability model**

The dual-permeability model represents the matrix as a continuum, for which we can obtain a similar set of equations as those for the fractures

\[
\frac{\partial (\phi^m s^m c)}{\partial t} + \nabla \cdot \mathbf{u}^m = q^f_{c^m} + \psi^m_c,
\]

(6.7)

\[
\frac{\partial (\phi^m s^m b)}{\partial t} + \nabla \cdot \mathbf{u}^m = q^f_{b^m} + \psi^m_b,
\]

(6.8)

where the phase fluxes \( \mathbf{u}^m_c \) and \( \mathbf{u}^m_b \) are

\[
\mathbf{u}^m_c = -\frac{k^m_{r,c} k^m_c}{\mu_c} (\nabla p^m_c - \rho_c \mathbf{g}),
\]

(6.9)

\[
\mathbf{u}^m_b = -\frac{k^m_{r,b} k^m_b}{\mu_b} (\nabla p^m_b - \rho_b \mathbf{g}).
\]

(6.10)
Modified dual-permeability model

The dual-permeability model can be modified to a “match-stick” model (Gilman and Kazemi [1988], Kazemi and Gilman [1993]), where only vertical flow is considered in the matrix domain. The “match-stick” model represents a highly fractured system with only vertical fractures. The mass balance equations for CO$_2$ and brine in the matrix can be obtained

$$\frac{\partial (\phi^m s^m_c)}{\partial t} + \frac{\partial u^{m,c}_z}{\partial z} = q^{f-m}_c + \psi^m_c,$$

$$\frac{\partial (\phi^m s^m_b)}{\partial t} + \frac{\partial u^{m,b}_z}{\partial z} = q^{f-m}_b + \psi^m_b,$$

where $u^{m,c}_z$ and $u^{m,b}_z$ denote the phase fluxes of CO$_2$ and brine, respectively, in the vertical direction (assumed positive upward).

The phase fluxes can be computed with the fractional flow formulations

$$u^{m,c}_z = \frac{\lambda^m_c}{\lambda^m_c + \lambda^m_b} (u_{tot,z}^m + \lambda^m_b k^m \Delta \rho g - \lambda^b_b \nabla p^{cap.m}),$$

$$u^{m,b}_z = \frac{\lambda^m_b}{\lambda^m_c + \lambda^m_b} (u_{tot,z}^m - \lambda^m_c k^m \Delta \rho g + \lambda^c_c \nabla p^{cap.m}),$$

where $\lambda^m_c$ and $\lambda^m_b$ are the phase mobilities for CO$_2$ and brine in the matrix, respectively; $\Delta \rho = \rho_b - \rho_c$ represents the density difference.

The total flux $u^{m, tot}_z$ can be obtained by summing Equations (6.11) and (6.12), where we obtain

$$\frac{\partial u^{m, tot}_z}{\partial z} = q^{f-m}_c + q^{f-m}_b + \psi^m_c + \psi^m_b.$$

Equations (6.11) to (6.14) form a complete set of equations for the “match-stick” model for the matrix flow.
Mass transfer function

The key component of the dual-porosity and dual-permeability models is the mass transfer function that governs the fluid exchange between the fractures and the matrix domain. The transfer function in general should account for imbibition, gravity drainage, capillary pressure, fluid expansion and molecular diffusion. For the CO$_2$ - brine system, we use the mass transfer function from [Ramirez et al. (2009)] that considers capillary pressure and gravity drainage, and has a functional form for the CO$_2$ flux from fracture to matrix as

$$q_{c}^{f-m} = \sigma k^{m} \frac{\lambda_{c}^{m}}{\lambda_{c}^{f} + \lambda_{b}^{m}} \left[ -(p_{\text{cap},m} - p_{\text{cap},f}) + \frac{\sigma_{z}}{\sigma} \Delta \rho g \left( \frac{s_{c}^{f} - s_{cr}}{1 - s_{cr}} - \frac{s_{c}^{m} - s_{cr}}{1 - s_{cr}} \right) L_{z} \right], \quad (6.16)$$

where $\sigma$ is the shape-factor of a matrix block, $\sigma_{z}$ is the component of $\sigma$ considering only the vertical direction, $L_{z}$ is the vertical dimension of a matrix block, $s_{cr}^{f}$ and $s_{cr}^{m}$ are residual CO$_2$ saturations in the fracture and the matrix, respectively. The shape-factor of a matrix has a number of expressions in the literature ([Ramirez et al. 2009]). Here, we introduce a simple expression from [Kazemi et al. (1992)]

$$\sigma = \frac{1}{V} \sum_{j=1}^{J} \frac{A_{j}}{d_{j}}, \quad (6.17)$$

where $A_{j}$ denotes the area for the open surface $j$ of the matrix block; $d_{j}$ is the distance from the center of the matrix block to the open surface $j$; $J$ represents the total number of open surfaces; and $V$ is the volume of the matrix block.

From $q_{c}^{f-m}$, we can obtain $q_{c}^{m-f} = -q_{c}^{f-m}$. Also, because we assume that the fluids are incompressible, $q_{b}^{f-m} = -q_{c}^{f-m}$. Therefore, from Equation (6.16), we can compute all the mass transfer terms $q_{c}^{f-m}$, $q_{c}^{m-f}$, $q_{b}^{f-m}$, and $q_{b}^{m-f}$.
### 6.2.2 Vertically-integrated modified dual-permeability model

The multiscale dynamic reconstruction framework developed in Chapters 4 and 5 can also be extended for dual-porosity and dual-permeability models for CO$_2$ sequestration in fractured reservoirs. Here, we take the modified dual-permeability model as an example and formulate a vertically-integrated model in the context of the multiscale dynamic reconstruction framework. In the modified dual-permeability model, because of the high permeability of fractures, the flow in fractures is likely to follow the vertical equilibrium assumption, for which we can use a vertical equilibrium model. In addition, the capillary pressure is likely to be small and therefore can be neglected, leading to a vertical equilibrium and sharp interface model. The matrix involves two-phase flows in a series of independent vertical columns and exchanges fluids with the fractures. In the context of a multiscale framework, the (vertically-integrated) vertical equilibrium model for fracture flow is the coarse-scale model, and the one-dimensional two-phase flow model in the columns represents a fine-scale model. This two-scale model is analogous to the multiscale dynamic reconstruction algorithm in chapter 4. The only difference is that here the two scales are coupled by the exchange of fluids, while the two scales in chapter 4 are coupled by the coarse-scale mobilities and the coarse-scale pressure.

On the coarse scale (fracture domain), we formulate the governing equations for flow of CO$_2$ and brine using the vertical equilibrium and sharp interface model. For a radial domain like Figure 2.1 in chapter 2, we can derive an equation for the height of the CO$_2$ plume \( h(r, t) \) as a function of the radial distance \( r \) and time \( t \) as

\[
\frac{\partial h^f}{\partial t} - \frac{1}{\phi r} \frac{\partial}{\partial r} \left( \frac{\Delta \rho g k h^f (h_0 - h^f)}{\mu_b h^f + \mu_c (h_0 - h^f)} \frac{\partial h^f}{\partial r} + \frac{q \mu_c (h_0 - h^f)}{2 \pi \mu_b h^f + \mu_c (h_0 - h^f)} \right) = \frac{1}{2 \pi \phi h_0} \int_0^{h_0} (q_{m-f} \psi_c) dz,
\]

(6.18)

where \( h_0 \) is the thickness of a geologic formation, which is assumed to be homogeneous and is characterized by the porosity \( \phi \) and permeability \( k \); residual saturations of CO$_2$ and brine are neglected, i.e., CO$_2$ saturation is 1 within the CO$_2$ plume and brine saturation...
is 1 outside the CO₂ plume. Equation (6.18) describes the CO₂ and brine migration in the fractures. It needs 1 initial condition and 2 boundary conditions. Initially, the geologic formation is filled with brine, thus the initial condition is $h^f(r, t = 0) = 0$. The two boundary conditions can be derived analogously as done in Chapter 2.

On the fine scale (matrix domain), we use Equation (6.11) to (6.15) to solve for the phase saturations of CO₂ and brine in the matrix. Initially, the matrix has no CO₂, thus the initial condition is $s^m_c(z, t = 0) = 0$ and $s^m_b(z, t = 0) = 1$. The two boundary conditions are no-flow conditions at the top and bottom of the geologic formation.

The set of two-scale equations (6.11) to (6.15) and (6.18) need to be solved numerically. Here, we briefly outline a numerical solution procedure to solve the two scales sequentially (see Table 6.1).

---

**Table 6.1: Numerical solution procedure for the vertically-integrated modified dual-permeability model**

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Compute $q_{m-f,n}$, solve for $h^{f,n+1}$ from Equation (6.18);</td>
</tr>
<tr>
<td>2.</td>
<td>From $q_{c}^{f-m,n} = -q_{c}^{m-f,n}$, solve for $u_{tot,z}^{m,n+1}$ from Equation (6.15);</td>
</tr>
<tr>
<td>3.</td>
<td>Compute $u_{c,z}^{m,n+1}$ from Equation (6.13);</td>
</tr>
<tr>
<td>4.</td>
<td>Compute $s^{m,n+1}_c$ from Equation (6.11) and obtain $s^{m,n+1}_b = 1 - s^{m,n+1}_c$.</td>
</tr>
</tbody>
</table>

---

**6.2.3 Summary**

In this section, we have briefly reviewed the various dual-porosity and dual-permeability models for CO₂ injection in fractured reservoirs. Taking the modified dual-permeability model as an example, we developed a vertically-integrated model in the context of the multiscale dynamic reconstruction framework from Chapters 4 and 5. Similar vertically-integrated formulations can be developed for the dual-porosity and dual-permeability mod-
els. We note that for the dual-permeability model, the dynamic reconstruction model needs to be applied to the matrix domain when the vertical equilibrium assumption is invalid. In this case, the vertically-integrated dual-permeability model will have two parts: a vertical equilibrium model for the fracture domain and a single-layer dynamic reconstruction model for the matrix domain. Further development of these models is part of some ongoing work.
Chapter 7

Summary and Conclusions

This dissertation reports studies on the multiphase flow dynamics of various subsurface systems that involve fluid injection and migration. It develops a set of computational models with different levels of complexity that have a broad range of applications, including geologic CO$_2$ sequestration, enhanced oil recovery, liquid waste disposal, and acid gas injection. Following is a summary of the core chapters (Chapters 2 to 6) of the dissertation.

In the first part of the dissertation (Chapters 2 and 3), we simplify the subsurface system with vertical equilibrium and sharp interface assumptions and develop a reduced-order model, i.e. the vertical equilibrium and sharp interface model, to understand the essential flow behaviors of the injection systems. Chapter 2 analyzes the vertical equilibrium and sharp interface model for an axisymmetric flow problem from fluid injection into a confined aquifer and obtains four analytical solutions at four asymptotic limits. Using these four asymptotic limits, we develop a flow regime diagram that depends on the viscosity ratio between the injected and displaced fluid and a buoyancy parameter that measures the relative importance between buoyancy and the driving force from injection. The flow regime diagram characterizes the flow behaviors of the injection system and identifies conditions under which each of the analytical solutions is appropriate. Chapter 3 uses the flow regimes to analyze practical fluid injection projects including geologic CO$_2$ sequestration.
enhanced oil recovery, liquid waste disposal, and acid gas injection. Such flow regime analysis provides insights for the flow processes and serves to guide the choice of simplified models and analytical solutions that can be applied to different kinds of injection scenarios.

In the second part of the dissertation (Chapter 4 and Chapter 5), we develop novel multiscale numerical algorithms and a range of vertically-integrated models that are capable of modeling the vertical two-phase flow dynamics of CO$_2$ and brine in homogeneous and layered heterogeneous geologic formations. These multiscale vertically-integrated models maintain much of the computational advantage of the conventional vertical equilibrium models, and therefore require much less computational efforts compared to full three-dimensional simulators. The capability to capture more physics while still maintaining a significantly reduced level of computational effort makes these multiscale models very attractive for computational studies of large-scale CO$_2$ storage systems, especially where the vertical dynamics of CO$_2$ and brine and vertical layered heterogeneity are important.

In the final part of the dissertation (Chapter 6), we outline two directions of extensions to develop more advanced models from the multiscale algorithm developed in Chapters 4 and 5. The first extension is a range of hybrid models that couple the different model options with different levels of complexities in the vertical direction, i.e. the hybrid multi-layer vertically-integrated models, and in the horizontal direction, i.e. hybrid multi-dimensional models. These hybrid models with carefully considered adaptivity criteria for switching between the different modeling options can be powerful computational tools to simulate large-scale complex multiphase flow systems. The second extension is the use of the multiscale framework to develop vertically-integrated dual-porosity dual-permeability models for CO$_2$ injection in fractured reservoirs. These multiscale models could provide computationally efficient modeling tools for CO$_2$ injection in fractured rocks.
Bibliography


Doughty, C., B. M. Freifeld, and R. C. Trautz (2008), Site characterization for CO$_2$ geologic storage and vice versa: the Frio brine pilot, Texas, USA as a case study, *Environ. Geol.*, 54(8), 1635–1656.


IPCC (2005), Metz, B., O. Davidson, H. De Coninck, M. Loos, and L. Meyer (Eds.), IPCC special report on carbon dioxide capture and storage, prepared by working group III of the Intergovernmental Panel on Climate Change.


Scripps Institution of Oceanography (2016), The keeling curve: A daily record of atmospheric carbon dioxide from the scripps institution of oceanography at UC San Diego.


