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Simulation of Flow in Porous Media

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Preface

This book consists of six invited expository chapters resulting from the workshop *Simulation of Flow and Transport in Porous Media and Applications in Waste Management and CO_2 Sequestration* which took place on October 3–7, 2011, at the Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences, Linz, Austria. This workshop with 21 invited speakers and more than 60 participants was part of a special semester on *Multiscale Simulation and Analysis in Energy and Environment* that took place between October 3 and December 16 at RICAM with a total of about 200 participants (Chair: R. Scheichl). The goal of the special semester was to stimulate interdisciplinary cooperation between engineers, hydrologists, meteorologists, and mathematicians for these highly important societal problems. It consisted of four focused workshops and a large visitors program, with long-term visitors interacting with RICAM staff and with each other, including graduate courses and "research kitchens."

The workshop, from which the present chapters arose, focused on mathematical and computational issues in subsurface flow. Subsurface flow problems are inherently multiscale in space due to the large variability of material properties, as well as in time due to the coupling of many different physical processes, such as advection, diffusion, reaction, and phase exchange. Mathematical models for these processes still need considerable development. However, significant progress is crucial, in particular in energy and environmental applications, to successfully tackle such important societal challenges as long-term radioactive waste management and sequestration of CO_2 underground. The workshop focused on cutting-edge issues such as *multiphase flows* and *coupled problems*, and this book gives a cross section of the talks as well as the current state-of-the-art. The seemingly disparate, but equally timely topic of *fuel cell modeling* is mathematically very similar and so the workshop included a special session with three speakers also on that topic.

The chapters in this book are written by invited speakers and their collaborators and are intended to provide an overview of the topics covered by the workshop. The contributions may be grouped into two larger themes:

(1) *Multiphase Flow.* The chapter of S. Gasda et al. treats upscaling aspects of CO_2 sequestration in realistic geologic settings. M. Wolff et al. concentrate on accurate discretization schemes for multiphase flow on nonorthogonal meshes. A. Bourgeat et al. present results of a benchmark study in the context of nuclear waste storage.

(2) *Coupled Problems.* The mathematical and computational aspects of coupling surface or free flow with subsurface flow are addressed by the contribution of M. Discacciati. The contribution of J. Fuhrmann resulted from a special session on fuel cell modeling and gives an overview of mathematical and computational aspects of electrochemical devices. Last but not least the contribution of B. Ganis and coworkers covers multiscale aspects of coupled flow and geomechanics.

First and foremost, we thank all the authors of the chapters for sacrificing their valuable time to help us produce this exciting book. We would like to thank the former Director of RICAM, Prof. Heinz Engl, and the current Director, Prof. Ulrich Langer, for the invitation and for the opportunity to organize this special semester. We also want to particularly thank the administrative team at RICAM around Susanne Dujardin, Annette Weihs, Wolfgang Forsthuber, and Florian Tischler, as well as the local scientific organizers Joerg Willems, Johannes Kraus, and Erwin Karer. The special semester, the workshops, and this book would not have been possible without their efforts and commitment. A great thank you is also in order for the remaining members of the Program Committee, Mike Cullen (UK Met Office), Melina Freitag, Ivan Graham (both University of Bath), and Markus Melenk (TU Vienna). Finally we also thank the speakers and participants at the workshop for making it such an outstanding event.

More information on the special semester and the four workshops can be found at

http://www.ricam.oeaw.ac.at/specsem/specsem2011/

Bath — *Robert Scheichl*
Heidelberg — *Peter Bastian*
Linz — *Johannes Kraus*
Austin — *Mary Wheeler*

Contents

Sarah E. Gasda,Elsa du Plessis, and Helge K. Dahle

Upscaled models for CO_2 injection and migration in geological systems

Abstract: Geological sequestration of CO_2 may be an important tool to reduce anthropogenic emissions of greenhouse gases. To predict the long-term fate of the CO_2 plume and ultimately reduce the risks involved in injecting vast amounts of supercritical CO_2 into underground formations, simulation studies are necessary. However, because of large temporal and spatial variations in scale, realistic scenarios based on modeling can only be achieved through semi-analytical or upscaling techniques.

In this chapter, we review progress and limitation of upscaling methods based on assuming vertical equilibrium in the two-phase flow system. Using dimensional groupings, we show that these formulations are adequate for conditions that will occur in many typical storage scenarios. We then review the inclusion of capillarity, dissolution, compressibility, and caprock topography into these models. We review some of the benchmarking that has been performed on these types of methods, and finally give some simulation results based on realistic storage conditions.

Keywords: Geological CO_2 Sequestration, Vertical Equilibrium, Capillary Fringe, Dissolution, Convective Mixing, Compressibility, Caprock Rugosity, Benchmarking, Upscaled Model, Dimensionless Group.

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1 Introduction

Storage of carbon dioxide (CO_2) in deep geological formations has been proposed as a viable technology to mitigate greenhouse gas emissions [7, 44]. In order for geological CO_2 storage to be successful, large volumes of CO_2 on the order of a billion metric

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tons annually must be stored reliably and efficiently for 1000 years or more [56]. Detailed modeling and numerical simulations will be required to evaluate the feasibility of potential sequestration sites, in particular models will be needed to predict the ultimate fate of the CO_2 plume and assess possible risks associated with the large-scale migration over long timescales [50].

In prospective sites for CO_2 storage, such as a saline aquifer or abandoned petroleum reservoir, the subsurface conditions are such that CO_2 is a supercritical fluid [4] and slightly soluble in water (the solubility limit is about 4% by volume [19]) and thus forms a separate fluid phase that is less dense and much less viscous than the resident brine [51]. This results in a two-phase flow system in which the injected CO_2 will spread radially away from the injection well and displace the brine, whereas buoyancy forces will cause CO_2 to move progressively higher in the formation. The upward movement of the CO_2 plume will typically be constrained by a low-permeability caprock that bounds the aquifer above.

Accurate and efficient models are required that can resolve the two-phase flow physics within very large spatial and temporal domains associated with CO_2 storage. In addition, other relevant aspects of CO_2 migration and trapping need to be captured. For instance, the migration of CO_2 can be affected by local capillary effects [53], the rock can deform due to thermomechanical stresses [59, 66], and CO_2 dissolution in brine can be enhanced by density-driven convection under the plume fringe [20]. Other salient processes include the creation of "wet" CO_2 due to evaporation of water into the CO_2-phase, a drying front behind the CO_2 injection front that corresponds to dry CO_2 in the formation [49], and salt precipitation [62], among others. This full suite of physical processes must be modeled given the heterogeneity and structural complexity typical of most sedimentary systems.

Numerous state-of-the-art modeling frameworks have been applied to CO_2 injection and storage in geological systems ([68] and references therein). Multipurpose numerical simulators for multiphase flow and transport in porous media, e.g. TOUGH2 [63] and ECLIPSE [67], allow for injection of CO_2 and modeling of heat and chemical species transport in heterogeneous three-dimensional geological systems. However, a significant challenge faced by traditional numerical approaches is the ability to resolve the relevant physics described above. This has been demonstrated in recent benchmark studies (e.g. [10]), where the task of providing spatially resolved, "full-physics" solutions in 3D proved to be inherently difficult. Part of the challenge is that gravity override leads to a very thin CO_2 fringe under the caprock, and resolving this fringe requires high vertical grid resolution; in particular, caprock topography, or roughness, have a strong impact on the distribution and areal extent of the CO_2 plume [28]. Likewise, the dynamics entails inherently unstable phenomena like convective dissolution [40, 57, 65] that necessitate highly resolved grids in the horizontal direction. The resolution requirements of these types of coupled systems are thus computationally intractable in large-scale CO_2-storage systems.

These computational challenges have led to the reemergence of upscaled models that resolve the physical processes in an average sense based upon depth integration. In this chapter, we present a review of recent advances in vertically integrated models and their application to CO_2 storage systems. We discuss the fundamental assumptions inherent in the vertically integrated approach and identify the range of validity of the model using several dimensionless groupings. The vertical equilibrium (VE) model equations are then formulated for the incompressible, immiscible case that accounts for non-linearities associated with capillary effects. The model is extended to account for subscale processes that may significantly impact CO_2 migration and trapping, including CO_2 compressibility, dissolution with convective mixing and subscale caprock roughness. Finally, several applications of the vertically integrated model are presented that show the practical benefits of the simplified modeling approach for real CO_2 storage systems.

2 Background

Large-scale and long-term storage of CO_2 in subsurface aquifers, as represented in Figure 1.1, presents a complex challenge in which multiple processes take place across various spatial and temporal scales. Including all of these processes over all relevant scales in a simulation to predict the long-term fate of the injected CO_2 leads to many complications, the result of which may not necessarily be an accurate prediction due to the inherit complexity of the entire system [49]. It is thus important to consider

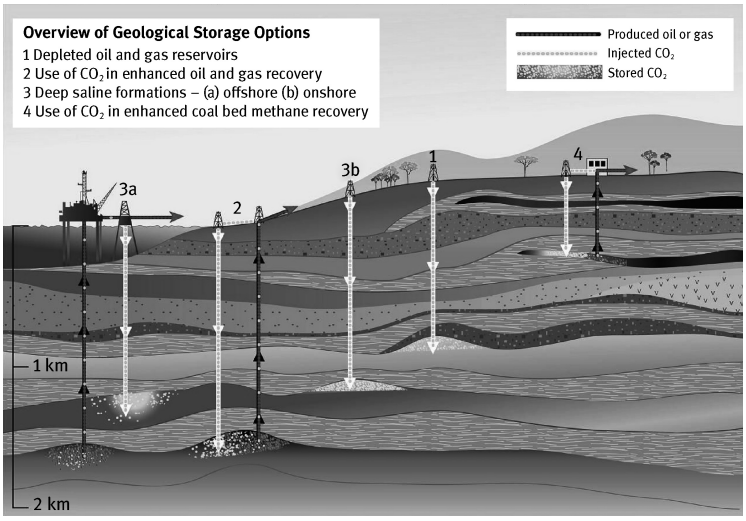

Figure 1.1: Storage of CO_2 in deep subsurface formations. Figure adapted from the IPCC report on carbon dioxide capture and storage [44].

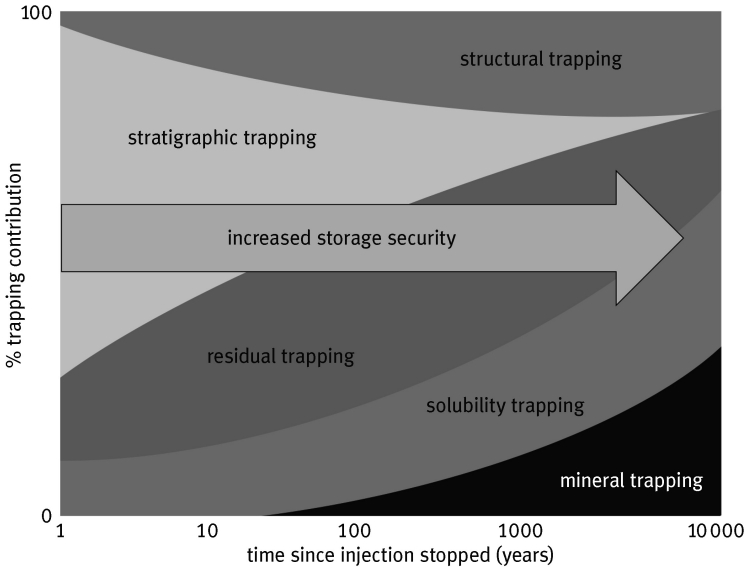

Figure 1.2: Schematic with the range of considered temporal scales with regards to increasing storage security in a CO_2-injection model. Figure adapted from the IPCC report on carbon dioxide capture and storage [44].

at which scales particular processes are dominant, and further, which processes are of most importance and which could possibly be considered negligible to simplify the modeling process.

Considerations across the spatial scales range from the interactions between CO_2 and brine at the pore scale, to the eventual lateral extent of both the CO_2 and pressure plumes on the aquifer scale. Similarly, temporal scale considerations range from the establishment of capillary equilibrium over a relatively brief timescale to the 1000-year timescale after which CO_2 is considered to be safely stored according to proposed guidelines [50]. Between both the extreme length and timescales are a multitude of other complex processes that may dominate over intermediate scales, which could in turn greatly affect plume-migration predictions.

Possible processes and model parameters affecting storage security across various timescales are represented in Figure 1.2. Immediately after injection, CO_2 is confined to the storage aquifer solely by stratigraphic or hydrodynamic trapping, e.g. a relatively impermeable caprock. As time progresses postinjection, residual trapping of CO_2, occurring on the pore scale, traps an increasing portion of CO_2 mass along with other interfacial behavior such as equilibrium partitioning. Over longer timescales, dissolution due to convective mixing [16] driven by centimeter-scale instabilities may act to enhance solubility trapping [16, 50]. Larger spatial scale considerations include the caprock topography [25], which could vary on the order of cen-

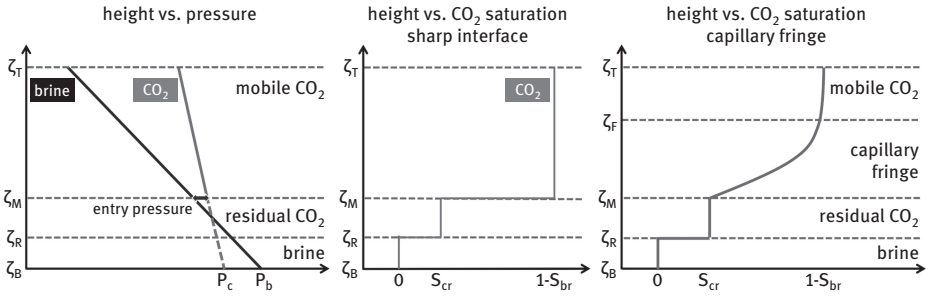

Figure 1.3: Pressure profiles of brine and CO_2 across the height of the aquifer under the VE assumption. Two different CO_2 saturation profiles correspond to the pressure profile (left) – a sharp interface assumption with abrupt saturation change at ζ_M (middle) and a capillary transition zone that leads to gradual saturation within the two-phase fringe (right).

timeters to meters yet may impact CO_2 migration over hundreds of kilometers. Such a phenomenon would lead to an increased amount of trapped of CO_2 at later times due to this structural heterogeneity. Mineral reactions that lead to mineral trapping occurs at the very lower end of the spatial spectrum and becomes increasingly important with regards to storage security at the far end of the temporal scale [50]. These slow reactions are separate from fast mineral reactions that may impact flow patterns near the injection well or enhance leakage along an old abandoned well.

The approach of using upscaling methods to simplify modeling of these large systems stems from taking advantage of the length scales relevant in geological systems which are deemed suitable for long-term storage of CO_2 [50]. Suitable sites under consideration for CO_2 injection are generally characterized by aquifers with a much greater horizontal span compared to the vertical. The proposed method is to reduce the dimensionality of the problem by upscaling the model parameters across the vertical span and to advance the solution across the horizontal extent of the aquifer, thus greatly reducing the computational cost.

Historically, it is exactly this computational cost of a full three-dimensional simulation that drove the development of upscaled models for fluid flow in reservoir simulations. Martin [43] proposed a mathematical framework whereby the equations for multiphase, three-dimensional compressible flow were reduced to a set of two-dimensional equations for the fluid flow in a reservoir through vertical integration of the model parameters. Importantly, the effects of fluid segregation due to density differences, as well as the effects of capillarity, which are both present across the vertical scale of a reservoir, were included in the simplified model. Martin's [43] framework built on and verified the work of Coats [11], in which the concept of VE was first introduced in reservoir engineering.

The crucial assumption of VE refers to a multiphase system in which the establishment of a pressure equilibrium across the vertical dimension occurs much faster

than the advancement of the actual saturation plume. The VE assumption translates into a system with negligible vertical flow and a hydrostatic pressure distribution of each phase, where gravitational and capillary forces are in equilibrium. Figure 1.3 represents the pressure profiles under the VE condition across the vertical extent of the aquifer of the resident brine and the injected CO_2, with quantities on the vertical axis denoting the respective interfaces in the system between the top and bottom of the aquifer. The pressure change in each phase is constant across the aquifer height which in turn implies that the change in capillary pressure is also constant across the aquifer height.

Given VE conditions, the upscaling techniques to obtain a mathematical VE model have historically started from the macroscale multiphase flow theory, including Darcy's law and local constitutive functions, i.e. relative permeability and capillary pressure relations. These three-dimensional equations are subsequently upscaled by integrating across the storage formation thickness. Alternative approaches have been suggested, such as the method developed by Gray et al. [29] which proposes direct integration from the microscale to the vertically integrated scale, a more complete derivation and one that can be constrained by thermodynamic relations of the system. This derivation has been applied previously to CO_2 storage systems [28].

The historical work of Martin [43] and Coats [11] came at a time when computational capabilities were very limited, making full scale reservoir simulation in especially the petroleum engineering industry [12, 14, 38] particularly challenging. Since then computational power and numerical methods have progressed significantly, yet the method of upscaling and the assumption of VE is still relevant and useful today. Such models are quite common in physics [33] but have enjoyed renewed interest in recent years with application to CO_2 injection into saline aquifers [30, 31, 37, 54]. Simplified models have recently been used in combination with Monte Carlo techniques [49, 51, 52] to assess leakage risks when a CO_2 plume contacts thousands of abandoned wells, a task that would be impossible to perform using standard simulation techniques. Likewise, analytical solutions for CO_2 gravity currents have been developed [31–33, 37, 42] to enable simplified calculations of the CO_2 inventory (free-phase CO_2, residual trapped CO_2, and possibly dissolved CO_2).

The reliability of these simplified models has been tested in a recent benchmark study [10], where an application of a VE model [22] to the Johansen formation produced qualitatively comparable results to those obtained by commercial codes resolving the full three-dimensional problem. A study on the application of a VE model to the Utsira formation [48] revealed that the simplified model could deliver more accurate results when full fluid segregation had taken place compared with a fully three-dimensional ECLIPSE simulation. In addition, the VE simulation proved to be significantly faster, and have thus proved to be an effective means to test different model choices and explore parameter spaces.

Vertical equilibrium models certainly have restrictions in their applicability and as such should not be expected to provide accurate results through all phases of CO_2

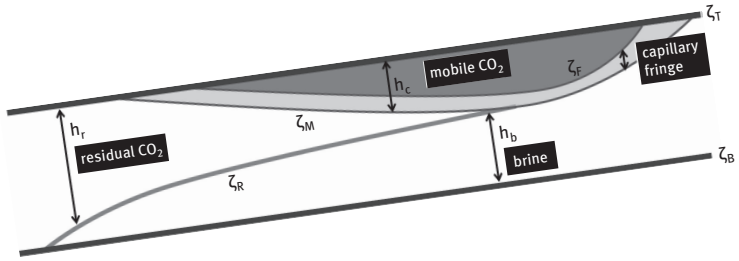

Figure 1.4: Sharp interface model with heights of brine, mobile CO_2, and residually trapped CO_2.

injection and storage [41]. As previously discussed, these models were developed for segregated fluids. In modeling the spread of a CO_2 plume, it should thus be noted that vertical fluid segregation due to the density difference of brine and supercritical CO_2 may not occur immediately and uniformly across the plume. The influence on vertical flow in highly anisotropic geological systems should also be considered, as these effects would not necessarily be captured by a simplified VE model. Various dimensionless groupings, discussed in more detail later, allow the specific system and spatial/temporal scales of interest to be analyzed and determine whether the fundamental assumptions of equilibrium are valid. In general, the VE model formulation is often better suited for predicting the long-term migration of injected CO_2 in reasonably heterogeneous aquifers where buoyancy effects are strong and the aspect ratio is high. Application during the injection phase is also suitable if the viscous-dominated region near the injection well is small and/or the near-well flow dynamics are not of primary interest.

Current VE models have been developed through integration of governing equations written at the Darcy scale (macro scale) and upscaled to the aquifer scale [50]. It is at this scale where results pertaining to the migration of the CO_2 plume are of interest. At the macroscale the equations for multiphase flow are written in terms of the respective saturations. The large aspect ratio of the aquifer may then be exploited in upscaling of the macroscale model, where the saturations are modeled as heights of the layers of each phase as in Figure 1.4. In this model it has been assumed that the interfaces between the phases are sharp [50]. The CO_2 plume is traveling up-slope above the resident brine in this formation, leaving a trail of residually trapped CO_2 in its wake. The simplicity of this model greatly reduces computational cost, and yet, as demonstrated by Nilsen et al. [48], delivers quantitatively accurate results when compared with commercial codes that resolve the fully three-dimensional scenario.

A simplified model such as the one depicted in Figure 1.4 could be extended to include more complex behavior in the system, depending on the primary goal of the simulation. It is possible to include effects of dynamic processes on the microscale by keeping track of changes in all three dimensions and upscaling again [50]. Through such a method there is continuous multiscale communication, ensuring that

any significant changes on the finer scale influence the upscaled model appropriately. Fine scale processes that could impact the eventual plume migration include relative permeabilities, the formation of a capillary fringe [53] and hysteretic effects.

The basic VE model starts off assuming a two-phase, immiscible system with a sharp interface and a regular, heterogeneous aquifer. Recent developments in increasing the complexity of this model include modeling the capillary fringe [53] and different trapping mechanisms within the system. Structural trapping, whereby pockets of CO_2 could potentially be immobilized and trapped between irregularities at the caprock interface, has been shown to be significant [25, 48]. In addition, Mykkeltvedt and Nordbotten [45] have studied the effects of convective mixing on the plume migration.

The development of simulators that implement the VE model is part of ongoing work. Because the simplified 2D model equations are analogous to the full three-dimensional system but with different definitions of the coarse-scale variables and constitutive functions, many of the same numerical methods can be applied to the VE model. Further developments have been made regarding the computational implementation of VE models, with the open-source MATLAB Reservoir Simulation Toolbox (MRST), developed by Nilsen et al. [48] available as an alternative to existing commercial codes [69]. The key focus in numerical implementation is on increasing efficiency. Although a key factor in efficiency is having fewer equations in a reduced dimension system, the VE model also weakens the pressure-transport coupling and eliminates the timestep restrictions that result from vertical resolution of sharp fronts required in 3D codes [34].

3 Model description

We describe the development of a simplified model for CO_2 injection, migration and trapping into a storage formation. The storage formation, which is defined as either the thickness of an entire permeable formation or of one stratified layer created by vertical heterogeneity in the formation, is initially saturated with brine and is bounded above and below by relatively impermeable shale formations. As depicted in Figure 1.4, the top and bottom boundaries are described by depth surfaces $\zeta_T = \zeta_T(x, y)$ and $\zeta_B = \zeta_B(x, y)$, respectively. In general, the storage formation may be heterogeneous with respect to geometry and other geological parameters.

We consider CO_2 injection into the storage formation as a two-phase two-component system. The CO_2-rich phase is denoted by subscript c whereas the brine-rich phase is denoted by subscript b. CO_2 migration is driven predominantly by gravity and viscous forces. CO_2 trapping occurs by three predominant mechanisms – structural trapping in local traps and domes, residual trapping due to capillary snap-off during imbibition, and solubility trapping due to CO_2 dissolution into the resi-

dent brine. We do not consider mineralization trapping, which occurs on a longer timescale than of interest.

The key aspects of the model development are integration over the vertical dimension of the storage formation and the simplifying assumptions associated with this upscaling procedure. Vertical integration is an upscaling step that coarsens the fine-scale model from three dimensions to two lateral dimensions. Thus, the "fine-scale" is defined as the full three-dimensional model that resolves the vertical dimension, while the "coarse-scale" is a two-dimensional model that represents the fine-scale vertical distribution with coarse-scale or average variables. We note that the horizontal scale of the fine- and coarse-scale models may be the same. Simplifying assumptions are needed to define coarse-scale variables as a function of fine-scale quantities and to reconstruct the solution at the fine scale if desired.

The simplified model derivation from three-dimensional REV-scale equations is described in this section. However in previous work, the VE model has been derived from the microscale directly to the depth-integrated scale [28]. To begin, we will summarize the conceptual framework as well as identify and describe the assumptions employed in the coarse-scale model development. These assumptions are not necessary for integration of the three-dimensional equations and may be relaxed depending on the system of interest.

3.1 Key assumptions and dimensionless groupings

The key assumptions for application of the VE model are as follows:

- large aspect ratio of the storage system;
- strong buoyancy effects;
- capillary–gravity equilibrium; and
- aquifer with modest heterogeneity and dip angle.

The necessary attributes of the storage system will be explored further here.

The first element of vertical integration is the assumption of VE at the fine scale. VE implies that pressure is in fluid-static equilibrium and vertical flow can be neglected. Fundamentally, VE requires a system with a large aspect ratio, i.e. the horizontal length scale (L) is significantly greater than the vertical (H) [70]. To determine the validity of VE for a given system, a dimensionless grouping can be formed using the aspect ratio and the permeability anisotropy ratio k_H/k_V

$$R_L^{-1} = \frac{H}{L}\sqrt{\frac{k_H}{k_V}}. \tag{1.1}$$

VE is a valid assumption when $R_L \gg 1$.

The VE assumption for a system with two fluids of different density implies fluid segregation due to gravity within a relatively short time. A dimensionless timescale

for gravity segregation can be formulated [53] as

$$T_v = T\,\frac{\lambda_c^* k_V \Delta\rho g \cos\theta}{\phi H}\,, \tag{1.2}$$

which consists of the density contrast between the two fluids $\Delta\rho = \rho_b - \rho_c$, gravitational constant g, endpoint CO_2 mobility at residual brine saturation λ_c^*, characteristic time T of the modeled system, vertical permeability k_V, porosity ϕ, formation dip angle θ and formation thickness H. We may assume complete gravity segregation within the timescale of interest when $T_v \gg 1$. There may be regions of the system where $T_v \ll 1$ due to strong viscous forces, e.g. close to the injection well. However, if vertical segregation has occurred over the majority of the plume, then the VE model may be applied during injection. When near-well dynamics are of primary interest then either a 3D model or some other upscaling/coupling techniques are required.

In addition to gravity forces, we must also consider capillary forces that act to disperse the two fluid phases over some characteristic length scale. Contrary to gravity, which forces the lighter fluid to be on top of the denser fluid, local capillarity disperses the lighter fluid downward and forms a transition zone, or capillary fringe, within which both fluids exist and are mobile. At equilibrium, the capillary and gravity forces are balanced, and the local distribution of saturation within the capillary fringe are fixed according to the local capillary-pressure saturation curve. The fringe has a dimensionless length scale ϵ [53],

$$\epsilon = \frac{p_c^*}{\Delta\rho g \cos\theta H}\,, \tag{1.3}$$

where p_c^* is the characteristic capillary pressure from the local p_c function for a given system. When $\epsilon \ll 1$ the fringe is relatively small and can be neglected, while when $\epsilon \gg 1$, then the transition zone is large and should be captured by the upscaled model.

The timescale to establish a capillary fringe (at capillary–gravity equilibrium) can be described by the dimensionless time [53],

$$T_f = T\frac{k_V}{\phi}\,\frac{\lambda_c^*\lambda_b^* p_c^*}{(\lambda_c^* + \lambda_b^*)(\epsilon H)^2}\,. \tag{1.4}$$

This timescale of vertical movement may be compared to the timescale associated with horizontal flow T_h,

$$T_h = T\frac{\lambda_c^* k_H \Delta\rho g \sin\theta}{H\phi(1 - s_{\mathrm{br}})} \tag{1.5}$$

with the residual brine saturation denoted as s_{br}. We may assume a capillary fringe has been established when the $T_f \gg 1$ and $T_h/T_f \ll 1$.

The final aspect is related to variation in caprock topography below some prescribed scale of the model resolution. The caprock roughness acts to retard CO_2 migration and increase subscale structural trapping. The strength of caprock roughness

factor decreases as the capillary fringe thickness increases. A dimensionless grouping indicates when one subscale process dominates over the other

$$R_c = \frac{p_c^*}{aH\Delta\rho g}, \tag{1.6}$$

where a is the characteristic amplitude of the underlying roughness scaled by aquifer thickness H. When $R_c \gg 1$, the capillary fringe has a dominant impact on CO_2 migration, while roughness dominates when $R_c \ll 1$.

Together these dimensionless groupings allow us to evaluate the types of systems, as well as the appropriate length and timescales, for which the VE and gravity-capillary equilibrium assumptions are valid. Taking the first dimensionless grouping R_L, we find that many prospective storage sites for CO_2 sequestration have large aspect ratios. For instance in the Alberta Basin in Western Canada, each potential storage formation in the geological sequence is tens to a few hundred meters thick, while the areal extent of each layer is several hundred kilometers in each direction [1]. When considering the large spatial extent that must be modeled for industrial-scale CO_2 injection, on the order of 100 km^2 or more, then R_L^{-1} will be significantly less than unity.

When considering gravity segregation, we observe that typical CO_2–brine systems across a wide range of temperature and pressure regimes will have short timescale to segregation relative to the timescale of interest. For example, a cold-deep aquifer will have density contrast of $350–400\,kg/m^3$, while at the other extreme, a warm-shallow aquifer will have a much larger contrast of up to $800\,kg/m^3$ [3]. Another example is the Utsira formation [9], where a high permeability and strong density contrast lead to gravity segregation on the order of days, or $T_f \simeq 10^{-2}$ if we are interested in years of simulation.

The analysis of a capillary fringe is more difficult because often the capillary pressure curves are not known or are only estimated for a given storage formation. However, given some commonly used capillary pressure parameters from CO_2 modeling studies in the literature [13], the time to establish a capillary fringe will be anywhere from days to months. Therefore, the timescale of the simulation should be long relative to this in order to assume capillary-gravity equilibrium.

We may also consider whether a sharp interface is a good assumption, in which case the type of capillary pressure function assumed becomes important. If a typical Brooks–Corey type of function is used [8], then a fringe thickness of tens of meters can be expected. Therefore, if the formation thickness is on the same order of magnitude as the fringe, then the fringe must be modeled. For formations over 100 m thick, the fringe often can be reasonably replaced with a sharp interface. As we will discuss, the vertically integrated model can incorporate both cases in the model formulation, however the sharp-interface model is a simpler derivation and implementation.

3.2 Vertical fluid and pressure distribution

If pressure and gravity–capillary equilibrium are established within a short timescale relative to the simulation time, then the fluids are segregated and a well-defined vertical fluid structure exists in the aquifer. As a result, the vertical space can be subdivided into macroscopic regions bound by macroscopic interfaces, as depicted in Figure 1.4. The topmost region is created during the drainage process as CO_2 displaces brine. Region 1 contains mobile CO_2 and is bounded at the top by the ζ_T interface and at the bottom by a dynamic macroscale interface at a depth defined by $\zeta_M(x, y, t)$ that evolves in space and time. During the drainage process, ζ_M will move downward, but when flow reverses and brine reimbibes the pore space, residual CO_2 is trapped behind the receding ζ_M interface. This creates a residual CO_2 region that is bound above by the ζ_M interface and below by another dynamic interface $\zeta_R(x, y, t)$. The bottommost region of fluid is the undrained brine region bound above by ζ_R and below by the aquifer bottom at ζ_B.

The mobile CO_2 region may be subdivided into two regions if a capillary fringe exists and $\epsilon \gg 1$. We can define a top subregion that contains only mobile CO_2 and residual brine, which corresponds to fully drained conditions. The second sub-region consists of the capillary fringe where both CO_2 and brine are mobile with a transition in saturation from endpoint CO_2 saturation to endpoint brine saturation. The two subregions are separated by another dynamic interface $\zeta_F(x, y, t)$, where $\zeta_M \leq \zeta_F \leq \zeta_T$.

Due to this well-defined vertical structure, the following relation between the macroscopic interfaces must hold for the VE model,

$$\zeta_B \leq \zeta_R \leq \zeta_M \leq \zeta_F \leq \zeta_T \,. \tag{1.7}$$

When $\epsilon \ll 1$, the capillary fringe region disappears and $\zeta_F = \zeta_M$ everywhere.

At equilibrium, pressure and saturation distributions in the vertical dimension are defined according to density and capillarity. For instance, a fluid-statics calculation can be used to derive a vertical pressure profile for each phase given a general fluid density profile $\rho_\alpha(z)$ and a single pressure P_α at some datum level, $z = \zeta_P$,

$$p_\alpha(z) - P_\alpha = \mathbf{e}_z \cdot \mathbf{g} \int_{\zeta_P}^{z} \rho_\alpha(z') \, \mathrm{d}z' \quad \alpha = c, b \,. \tag{1.8}$$

Here, we have chosen a coordinate system aligned with the large-scale aquifer dipping plane such that the $\mathbf{e}_z$ is the coordinate perpendicular to the plane. Thus, the gravitational vector becomes $\mathbf{e}_z \cdot \mathbf{g} = -g \cos\theta$. For an incompressible system, equation (1.8) becomes

$$p_\alpha(z) = P_\alpha - \rho_\alpha g \cos\theta (z - \zeta_P) \,, \tag{1.9}$$

which is depicted schematically in Figure 1.3. We note that there is no physical basis for defining the upscaled phase pressure at depths where the phase does not exist. However, in practice, the phase pressure can be extrapolated to the specified datum. Defining phase pressure in this way has no effect on the resulting model [53].

Given P_α as the upscaled phase pressure, we can define an upscaled capillary pressure

$$P_{\text{cap}}(x, y) = P_c(x, y) - P_b(x, y), \tag{1.10}$$

which can be related to the fine-scale capillary pressure p_{cap} as

$$p_{\text{cap}}[s_c(x, y, z)] = P_{\text{cap}}(x, y) + \Delta\rho g \cos\theta(z - \zeta_P). \tag{1.11}$$

Following [53], equation (1.11) can be used to reconstruct the fine-scale vertical saturation distribution $s_c(z)$,

$$s_c(z) = p_{\text{cap}}^{-1}\left[P_{\text{cap}} + \Delta\rho g \cos\theta(z - \zeta_P)\right]. \tag{1.12}$$

where p_{cap}^{-1} is the inverse of the fine-scale capillary pressure–saturation relationship. The p_{cap}–s function is dependent on the formation rock and fluid properties and must be obtained through laboratory experiments on core samples. If the samples are tested under ambient conditions, they must be rescaled to reservoir conditions before being applied in this model.

Given a p_{cap} function, calculation of the inverse is generally done numerically. During primary drainage, the inverse of the primary drainage curve is straightforward. However, during imbibition, the local saturation at the time of reversal $s_c^*(z)$ will dictate the imbibition or scanning curve that must be inverted to reconstruct the saturation distribution. Local residual saturations $s_{cr}(z)$ are also dependent on the reversal saturation.

In general, the vertical structure of fluids for systems with large capillary transition zones, i.e. $\epsilon \gg 1$, are shown in Figure 1.3 and can be written mathematically as

$$s_c(z) = \begin{cases} 0, & \text{if } \zeta_B \le z < \zeta_R \\ s_{cr}(s_c^*), & \text{if } \zeta_R \le z < \zeta_M \\ p_{\text{cap}}^{-1}, & \text{if } \zeta_M \le z < \zeta_F \\ 1 - s_{\text{br}}, & \text{if } \zeta_F \le z \le \zeta_T. \end{cases} \tag{1.13}$$

For the sharp-interface case ($\epsilon \ll 1$), the saturation distribution abruptly changes at the ζ_M interface with no transition zone (Figure 1.3). The mathematical description can then be greatly simplified as

$$s_c(z) = \begin{cases} 0, & \text{if } \zeta_B \le z < \zeta_R \\ s_{cr}^0, & \text{if } \zeta_R \le z < \zeta_M \\ 1 - s_{\text{br}}, & \text{if } \zeta_M \le z \le \zeta_T, \end{cases} \tag{1.14}$$

where s_{cr}^0 is the endpoint CO_2 residual saturation.