



13th International Conference on Greenhouse Gas Control Technologies, GHGT-13, 14-18
November 2016, Lausanne, Switzerland

Vertically integrated dual-porosity and dual-permeability models for CO₂ sequestration in fractured geological formation

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Abstract

Analysis of geological storage of carbon dioxide (CO₂) in deep saline aquifers requires computationally efficient mathematical models to predict the pressure evolution and the injected CO₂ plume migration. The subsurface system of CO₂ injection into saline aquifers can be modeled as a two-phase flow system, with a non-wetting less dense (supercritical) CO₂ phase and a denser brine as the wetting phase. For unfractured geological formations, one type of simplified model can be developed by integrating the three-dimensional governing equations in the vertical dimension. The vertically integrated models that assume buoyant segregation and vertical pressure equilibrium are referred to as vertical equilibrium (VE) models. VE models are computationally efficient owing to the dimension reduction from vertical integration, and have been extensively applied to field-scale modeling of CO₂ injection, migration, and leakage in the past decade. For fractured geological formations, it is challenging to directly use vertically integrated models, because CO₂ migration in fractured formations involves two different characteristic time scales due to significant contrast of permeability between the fractures and matrix. The high permeability of the fractures leads to fast buoyant segregation of CO₂ and brine in the vertical direction within the fractures, while lower permeability of the matrix typically leads to much slower flow dynamics that involve longer time scales for segregation.

In this paper, we use a dual-continuum approach to conceptualize the fractured geological formation, treating the fractures and the rock matrix blocks as overlapping continua, and develop vertically integrated models for CO₂ injection in fractured geological formation. We use a VE model for the fracture domain and explore different model options for the matrix domain, including the classical dual-porosity model that treats the matrix as a source/sink term for the fracture as well as other more advanced models that explicitly account for the two-phase flow dynamics

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of the CO₂ and brine in the matrix domain. We present the modeling framework and show preliminary model comparison results to demonstrate the applicability of the new models.

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Peer-review under responsibility of the organizing committee of GHGT-13.

Keywords: Vertically integrated models; dual-continuum models; CO₂ storage; fracture flow

1. Introduction

Safe and permanent geological storage of carbon dioxide (CO₂) requires prediction of CO₂ and brine migration as well as changes in fluid pressures. The subsurface system of CO₂ sequestration can be modeled as a two-phase flow problem, with a non-wetting less dense injected CO₂ phase and a wetting denser resident brine phase. When the geological formation has extensive fractures, the formation consists of high permeability fractures and a low permeability matrix. Mass exchange of CO₂ and brine between fractures and matrix leads to complex flow dynamics.

Fluid flows in fractured geological formations are often modeled with a dual-continuum approach that conceptualizes fractures and matrix blocks as two overlapping continua [1]. The early work of both [2] and [3] considered the fractures as a continuum. [2] 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. [3] 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. In this latter (dual-porosity) model, fluid in the matrix only exchanges with fluid in the fractures, and not directly with any adjacent matrix blocks. For both the dual-permeability and dual-porosity models, the transfer of mass between fractures and matrix is a 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. Many improvements have been made after the pioneering work of [2] and [3], especially in the development of the mass transfer functions. Recent reviews of various versions of the mass transfer functions can be found in [1] and [4].

With the dual-continuum conceptualization, modeling approaches for unfractured geological formations can be used for fluid flow in each of the two continua – fractures and matrix – for the fractured rock system. For unfractured saline aquifers, a set of so-called vertically integrated models has been developed. The dimension reduction resulting from vertical integration leads to very computationally efficient models. In the past decade, a range of vertically integrated models have been developed and applied to field-scale modeling of CO₂ injection, migration and leakage (see recent reviews [5-6]). Almost all of those models are based on the vertical equilibrium (VE) assumption, which assumes that the CO₂ and brine segregate rapidly in the vertical direction due to strong buoyancy, and the fluid phases are always in pressure equilibrium (hydrostatic) in the vertical dimension. Recently, more advanced vertically integrated models have been developed that explicitly represent two-phase flow dynamics in the vertical direction and therefore do not rely on the VE assumption [11-12]. For fractured geological formations, the high permeability of fractures leads to fast buoyant segregation of CO₂ and brine in the vertical direction, and therefore the VE model is likely to be applicable. Flow in the matrix is typically much slower and involves longer time scales for segregation; thus the VE approach is unlikely to apply in the matrix.

In this paper, we use a dual-continuum approach and develop vertically integrated models to simulate CO₂ injection and migration in fractured geological formations. We use a VE model for the fracture domain and explore different model options for the matrix domain, including the classical dual-porosity model that treats the matrix only as a source/sink term for the fracture, as well as other more advanced models that explicitly account for the two-phase flow dynamics of the CO₂ and brine in the matrix continuum. Corresponding vertically integrated mass transfer

functions are derived and used to model the mass exchange between the fracture and the matrix domains. We formulate equations for the different models and present preliminary results to demonstrate their applicability in terms of both accuracy and computational efficiency.

2. Three-dimensional dual-continuum models

In this section, we introduce governing equations for dual-porosity and dual-permeability models in a full multidimensional domain. We first present the equations for flow in fractures and then outline formulations for fluid flow in the matrix for different models, including dual-porosity, dual-permeability, and modified dual-permeability models.

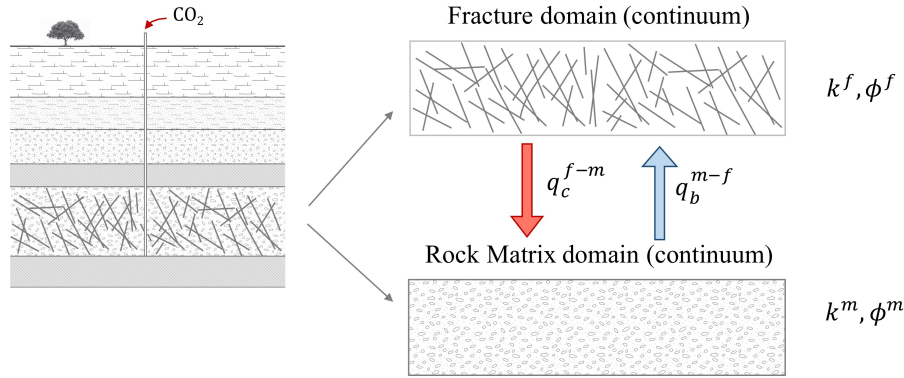


Figure 1: Schematic of a dual-continuum conceptualization of a fractured geological formation for CO₂ storage. The red and blue arrows denote CO₂ flux from fracture to matrix and brine flux from matrix to fracture, respectively. Both fracture and matrix domains are assumed to be homogeneous and isotropic with permeability k^f and porosity ϕ^f for the fracture domain, and permeability k^m and porosity ϕ^m for the matrix domain.

Both the dual-porosity model and the dual-permeability model consider the fractures as a continuum, where Darcy's Law applies for the fluid flow dynamics (Figure 1). For a homogeneous and isotropic fracture domain, we define ϕ^f and k^f as the porosity and permeability (assuming isotropic permeability), respectively, s_α^f the phase saturation, ρ_α the density of the fluid, and p_α^f the phase pressure. The superscript f denotes that the parameters are defined in the fracture domain, and the subscript $\alpha = c$ or b represents CO₂ ($\alpha = c$) or brine ($\alpha = b$). Assuming that CO₂ and brine are immiscible and incompressible, we can write mass balance equations for both the CO₂ and brine phases

$$\frac{\partial(\phi^f s_c^f)}{\partial t} + \nabla \cdot \mathbf{u}_c^f = q_c^{m-f} + \psi_c^f, \quad (1)$$

$$\frac{\partial(\phi^f s_b^f)}{\partial t} + \nabla \cdot \mathbf{u}_b^f = q_b^{m-f} + \psi_b^f, \quad (2)$$

where q_c^{m-f} and q_b^{m-f} represent CO₂ and brine volumetric fluxes from the matrix to the fracture domain, respectively; ψ_c^f and ψ_b^f denote the volumetric source terms of CO₂ and brine in the fractures, respectively; and the CO₂ and brine phase fluxes \mathbf{u}_c^f and \mathbf{u}_b^f can be obtained from extended Darcy's Law for two-phase flow

$$\mathbf{u}_c^f = -\frac{k_{r,c}^f k^f}{\mu_c} (\nabla p_c^f - \rho_c \mathbf{g}), \quad (3)$$

$$\mathbf{u}_b^f = -\frac{k_{r,b}^f k^f}{\mu_b} (\nabla p_b^f - \rho_b \mathbf{g}), \quad (4)$$

where $k_{r,c}^f$ and $k_{r,b}^f$ are relative permeabilities for CO₂ and brine, respectively; μ_c is viscosity for CO₂ and μ_b is viscosity for brine; \mathbf{g} is gravity acceleration vector.

The difference between the dual-porosity and the dual-permeability models lies in the flow model for the matrix. Dual-porosity models consider the matrix as composed of disconnected blocks that provide storage volumes but only exchange fluids with the fractures and not with adjacent matrix blocks. As such, there is no flow within the matrix at the continuum scale. In dual-permeability models, flow can occur within the matrix continuum, so the appropriate continuum equations for flow need to be written for both the fractures and the matrix. In the following subsections, we outline governing equations for the matrix domain for both dual-porosity and dual-permeability models, and also for a modified dual-permeability model.

2.1. Dual-porosity model

The dual-porosity model assumes that fluids are immobile (at the continuum scale) within the matrix and only exchange mass with the fracture domain. Thus, we obtain the following mass balance equations for the matrix domain

$$\frac{\partial(\phi^m s_c^m)}{\partial t} = q_c^{f-m} + \psi_c^m, \quad (5)$$

$$\frac{\partial(\phi^m s_b^m)}{\partial t} = q_b^{f-m} + \psi_b^m, \quad (6)$$

where superscript m denotes that the variables are defined in the matrix domain; q_c^{f-m} and q_b^{f-m} are CO₂ and brine volumetric fluxes from the fracture domain to the matrix domain, respectively; ψ_c^m and ψ_b^m are the volumetric source terms of CO₂ and brine in the matrix domain. We note that by definition $q_c^{f-m} = -q_c^{m-f}$ and $q_b^{f-m} = -q_b^{m-f}$.

2.2. Dual-permeability model

The matrix domain has a non-zero permeability at the continuum level in the dual-permeability model, so that fluid flows in the matrix are governed by a similar set of equations as those in the fractures

$$\frac{\partial(\phi^m s_c^m)}{\partial t} + \nabla \cdot \mathbf{u}_c^m = q_c^{f-m} + \psi_c^m, \quad (7)$$

$$\frac{\partial(\phi^m s_b^m)}{\partial t} + \nabla \cdot \mathbf{u}_b^m = q_b^{f-m} + \psi_b^m, \quad (8)$$

where the phase fluxes \mathbf{u}_c^m and \mathbf{u}_b^m are

$$\mathbf{u}_c^m = -\frac{k_{r,c}^m k^m}{\mu_c} (\nabla p_c^m - \rho_c \mathbf{g}), \quad (9)$$

$$\mathbf{u}_b^m = -\frac{k_{r,b}^m k^m}{\mu_b} (\nabla p_b^m - \rho_b \mathbf{g}). \quad (10)$$

2.3. Modified dual-permeability model

The dual-permeability model can be modified to a simpler model, the so-called “match-stick” model [7-8], where the matrix is conceptualized as a collection of vertical columns separated by fractures (“match sticks”) and thus only vertical flow is considered in the matrix domain. The “match-stick” model represents a fractured system with (primarily) only vertical fractures. The mass balance equations for CO₂ and brine in the matrix can then be simplified to one space dimension,

$$\frac{\partial(\phi^m s_c^m)}{\partial t} + \frac{\partial u_{c,z}^m}{\partial z} = q_c^{f-m} + \psi_c^m, \quad (11)$$

$$\frac{\partial(\phi^m s_b^m)}{\partial t} + \frac{\partial u_{b,z}^m}{\partial z} = q_b^{f-m} + \psi_b^m. \quad (12)$$

where $u_{c,z}^m$ and $u_{b,z}^m$ denote the phase fluxes of CO₂ and brine, respectively, in the vertical direction (assumed positive upward).

The phase fluxes can also be written using the fractional flow formulation with no explicit presence of the phase pressures

$$u_{c,z}^m = \frac{\lambda_c^m}{\lambda_c^m + \lambda_b^m} (u_{\text{tot},z}^m + \lambda_b^m k^m \Delta \rho g - \lambda_b k \nabla p^{\text{cap},m}), \quad (13)$$

$$u_{b,z}^m = \frac{\lambda_b^m}{\lambda_c^m + \lambda_b^m} (u_{\text{tot},z}^m - \lambda_c^m k^m \Delta \rho g + \lambda_c k \nabla p^{\text{cap},m}), \quad (14)$$

where $\lambda_c^m = k_{r,c}^m / \mu_c$ and $\lambda_b^m = k_{r,b}^m / \mu_b$ are the phase mobilities for CO₂ and brine, respectively; $\Delta \rho = \rho_b - \rho_c$ is the density difference between the two fluid phases; $u_{\text{tot},z}^m = u_{c,z}^m + u_{b,z}^m$ is the vertical total flux, and $p^{\text{cap},m}$ is the capillary pressure. Again, for all terms, superscript m denotes quantities defined in the matrix.

Summing Equations (11) and (12) we obtain

$$\frac{\partial u_{\text{tot},z}^m}{\partial z} = q_c^{f-m} + q_b^{f-m} + \psi_c^m + \psi_b^m. \quad (15)$$

If the top and the bottom boundaries of the geological formation are assumed impermeable, $u_{\text{tot},z}^m$ should be zero along the vertical column of the matrix, leading to counter-current flows with source and sink terms in the matrix columns.

2.4. Mass transfer function

The key component of dual-porosity and dual-permeability models is the mass transfer function that governs the fluid exchange between fractures and matrix. The transfer function in general should account for various physical mechanisms including imbibition, gravity drainage, capillary pressure, fluid expansion and molecular diffusion. In practice, simplified versions that capture some of the mechanisms are usually used. In this paper, we adopt mass transfer functions from the literature.

For the dual-porosity model, we use the mass transfer function from [1] that considers capillary pressure and gravity drainage, and has a functional form for the CO₂ flux from fracture to matrix as

$$q_c^{f-m} = \sigma k^m \frac{\lambda_c^f}{\lambda_c^f + \lambda_b^m} \left[-(p^{\text{cap},m} - p^{\text{cap},f}) + \frac{\sigma_z}{\sigma} \Delta \rho g \left(\frac{s_c^f - s_{c,r}^f}{1 - s_{c,r}^f} - \frac{s_c^m - s_{c,r}^m}{1 - s_{c,r}^m} \right) L_z \right], \quad (16)$$

where σ is a shape-factor for the rock matrix block, and σ_z is the component of σ considering only the vertical direction; L_z is the height of a matrix block; and $s_{c,r}^f$ and $s_{c,r}^m$ are residual CO₂ saturations in the fracture and the matrix, respectively. The shape-factor for the rock matrix block has a number of expressions in the literature [1]. Here, we introduce a simple expression from [9]

$$\sigma = \frac{1}{V} \sum_{j=1}^J \frac{A_j}{d_j}, \quad (17)$$

where A_j denotes the area for the open surface j of a rock 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, $q_b^{m-f} = q_c^{f-m}$. Therefore, from Equation (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} .

For the dual-permeability model, we use the mass transfer function from [10]

$$q_c^{f-m} = \sigma k^m \left[\left(\frac{k_{r,c}}{\mu_c} \right)^f \delta + \left(\frac{k_{r,c}}{\mu_c} \right)^m (1 - \delta) \right] \left[p_b^f - p_b^m + p^{cap,f} - p^{cap,m} + \frac{\sigma_z}{\sigma} \Delta \rho g \left(\frac{s_c^f - s_{c,r}^f}{1 - s_{c,r}^f} - \frac{s_c^m - s_{c,r}^m}{1 - s_{c,r}^m} \right) L_z \right], \quad (18)$$

where δ is the upstream weighting indicator that is 1 when CO₂ flux is from fracture to matrix, and equals to 0 otherwise. The transfer function term q_b^{m-f} can be derived in a similar fashion. Note that q_b^{m-f} is not necessarily equal to q_c^{f-m} because the mass transfer function includes the driving force due to phase pressure difference from fracture and matrix, which might drive both CO₂ and brine from fracture to matrix.

3. Vertically integrated dual-continuum models

3.1. Vertical equilibrium model for the fracture domain

The fracture domain has high permeability where the buoyant segregation of CO₂ and brine is likely to be rapid and thereby a VE model may be a good approximation. In addition, because of large pores in the fracture the capillary pressure is likely to be small and therefore can be neglected, leading to a VE sharp interface model (Figure 2). Here, we formulate the governing equations of the VE sharp interface model for flow of CO₂ and brine in the fracture domain.

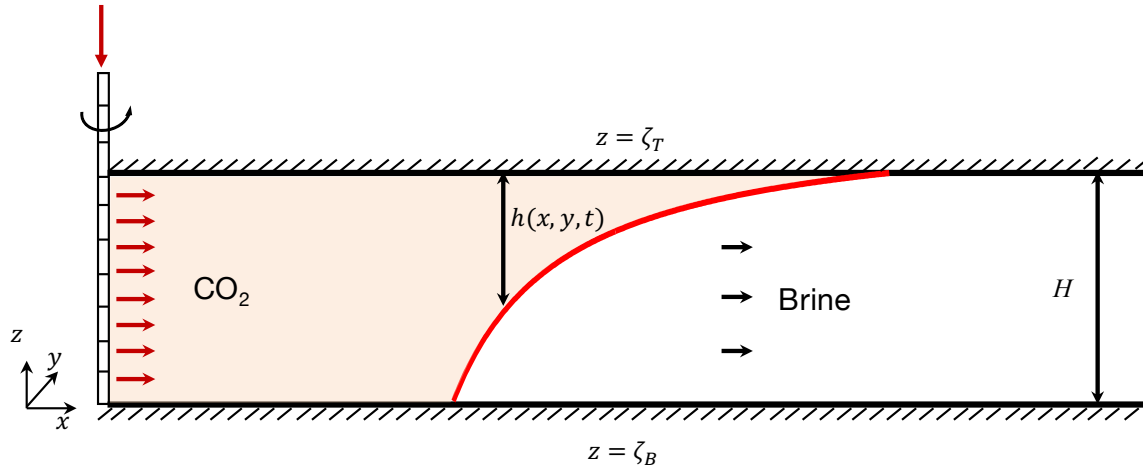


Figure 2: Schematic of the VE sharp interface model in the fracture domain. $z = \zeta_T$ and $z = \zeta_B$ are the top and the bottom boundaries of the geological formation respectively, and $H = \zeta_T - \zeta_B$ is the thickness of the formation; $h(x, y, t)$ is the thickness of the CO₂ plume; the red line denotes the macroscopic sharp interface between CO₂ and brine. To demonstrate the idea, here we assume that the formation is horizontal and homogeneous, although we recognize that the VE sharp interface model applies to formations with varying topography and heterogeneity.

In the VE sharp interface model, phase pressures of both CO₂ and brine are assumed hydrostatic. A pressure ($p_\alpha^f(x, y, z, t)$) at any point in space can be linked to the pressure ($P_\alpha^f(x, y, t)$) at the bottom of the formation as shown in Equation (19).

$$p_\alpha^f(x, y, z, t) = P_\alpha^f(x, y, t) - \rho_\alpha g z. \quad (19)$$

Due to the assumption of negligible capillary pressure in the fracture domain, CO₂ and brine in the fractures form a macroscopic sharp fluid-fluid interface. Here, we assume that the residual saturation of CO₂ and brine are both zero, although they can be easily included in the model. We integrate the mass balance Equations (1) and (2) for CO₂ and brine along the vertical direction from the bottom ($z = \zeta_B$) to the top of ($z = \zeta_T$) of the geological formation and obtain

$$\phi^f \frac{\partial h}{\partial t} - \nabla \cdot \left[\frac{k^f}{\mu_c} h (\nabla P_b^f + \Delta \rho g \nabla h) \right] = Q_c^{m-f} + \psi_c^f, \quad (20)$$

$$-\phi^f \frac{\partial h}{\partial t} - \nabla \cdot \left[\frac{k^f}{\mu_b} (H - h) \nabla P_b^f \right] = Q_b^{m-f} + \psi_b^f, \quad (21)$$

where

$$Q_c^{m-f} = \int_{\zeta_B}^{\zeta_T} q_c^{m-f} dz, \quad Q_b^{m-f} = \int_{\zeta_B}^{\zeta_T} q_b^{m-f} dz, \quad (22)$$

$$\psi_c^f = \int_{\zeta_B}^{\zeta_T} \psi_c^f dz, \quad \psi_b^f = \int_{\zeta_B}^{\zeta_T} \psi_b^f dz. \quad (23)$$

H is the thickness of the geological formation, and h is the thickness of the CO₂ plume in the fracture domain.

Summing Equations (20) and (21) gives a pressure equation for P_b^f . With the pressure equation in combination with Equation (20) (or Equation (21)), we can solve for the primary variables P_b^f and h using an IMPES (implicit pressure explicit saturation) method. We note that the phase pressure in the fracture is denoted by upper case letter P_b^f because it represents the bottom brine pressure defined in the vertically integrated set of governing equations (20) and (21), which are often referred to as coarse-scale equations and coarse-scale variables in a multiscale framework for vertically integrated models [13, 11]. The variables in the matrix are denoted by lower case letters, which correspond to the fine-scale variables [13, 11]. Different model options for the matrix flow lead to different pressure equations. For dual-permeability model, the mass transfer function q_α^{m-f} will depend on the fracture phase pressure (and therefore P_b^f) and the phase pressures in the matrix. The pressure equations for the fracture and the matrix are coupled through the mass transfer functions. For dual-porosity model, the mass transfer functions have no dependence on phase pressures, and the pressure equation thus only involves the phase pressure in the fracture domain.

3.2. Modeling options for the matrix domain

3.2.1. Dual-porosity

In the dual-porosity model, the mass transfer function does not depend on phase pressures of the two fluids. Thus, we locally compute the mass transfer function based on phase saturations (and capillary pressure), and then integrate the mass transfer function along the vertical direction to get Q_c^{f-m} and Q_b^{m-f} . The computation of phase saturation in the matrix is the same as the three-dimensional dual-porosity model.

3.2.2. Dual-permeability

The dual-permeability model is more complex than the dual-porosity model, because the mass transfer function depends on phase pressures, which leads to coupled pressure equations for the fracture and matrix domains. The pressure equation gives P_b^f and p_b^m , based on which we can solve the transport equation to get the CO₂ plume height h in the fracture, and s_c^m in the matrix.

3.2.3. Modified dual-permeability

For the modified dual-permeability model, we only need to consider the two-phase flow dynamics in the vertical dimension of the matrix domain. The mass transfer function from the dual-porosity that does not depend on phase pressures can be applied. We solve the one-dimensional columns using fractional flow equations that allow elimination of explicit presence of phase pressures. For impermeable top and bottom boundaries of the geological formation, the vertical total flux in the matrix is zero.

4. Results and discussion

Some of the models proposed in this paper are still under development; here we present some preliminary results. We first show that the VE sharp interface model is a good approximation for the two-phase flow dynamics in the fracture. To demonstrate that, we consider a two-dimensional (x - z) domain, and compare the VE dual-porosity model with a full 2D dual-porosity model. Figure 3 shows CO_2 saturation distributions in a fractured reservoir after five years of injection simulated by a VE dual-porosity model and a full 2D dual-porosity model. The horizontal length of the domain is 1500 m, and the thickness of the formation is 50 m. CO_2 is injected uniformly throughout the left boundary. Permeability and porosity are 100 mD and 0.05 for the fracture domain, and 1 mD and 0.15 for the matrix domain. Capillary pressure is set to zero for both fracture and matrix. The Brooks-Corey model with $\lambda = 2.0$ is used for the relative permeability of matrix in the mass transfer function. Numerical grid sizes of $\Delta x = 5$ m in x and $\Delta z = 0.2$ m in z are used for the full 2D dual-porosity model. The simulation results from the two models match well, measured by both the CO_2 plume extent and the mass fraction of CO_2 in the fracture and the matrix. The leading edge of the CO_2 plume in the fracture is 720 m from the VE dual-porosity model versus 575 m from the full 2D dual-porosity model, and the corresponding mass fraction of CO_2 in the matrix is 66.5% and 69.6%, respectively. We note that although the leading edge of the CO_2 plumes in the fracture domain has notable difference from the two models, the majority of the CO_2 plumes match well. We also point out that it is difficult to eliminate numerical diffusion in the vertical direction to accurately capture the CO_2 -brine sharp interface for the full 2D dual-porosity model; here we used $\Delta z = 0.2$ m. Much better match between the two models is expected for higher permeability of the fracture domain, because we used a fairly low permeability of 100 mD in this test case. Also, in our simulations, VE dual-porosity is at least two orders magnitude more computationally efficient than the full 2D dual-porosity model. This is because full 2D the dual-porosity model needs to solve a 2D pressure equation and requires very high vertical resolution to resolve the sharp interface and small time steps to capture the segregation process.

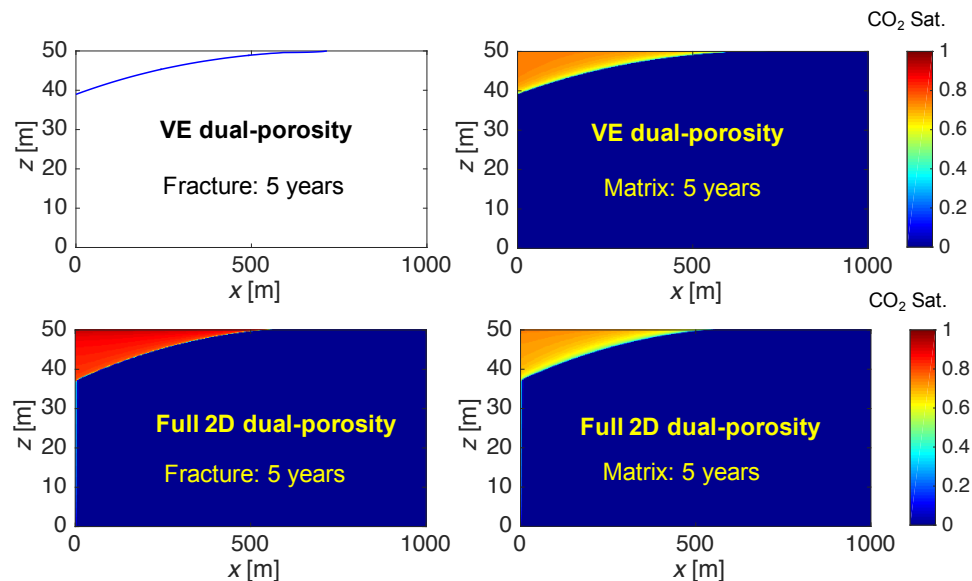


Figure 3: Simulation results of CO_2 distributions in a fractured geological formation using a VE dual-porosity model (top row) and a full 2D dual-porosity model (bottom row) after 5 years injection. The left plots are from the fracture domain and the right plots are from the matrix domain. The color scale denotes magnitude of CO_2 saturations from zero to one (residual saturations are neglected in the simulations), and the blue line in the left top plot denotes the sharp interface of CO_2 and brine.

In the second set of results, we show CO_2 distribution simulated by the VE dual-porosity model with different parameters in the mass transfer functions (Figure 4). Transfer functions with a lower and a higher rate are used, one

with $k^m = 0.1$ mD and the other with $k^m = 1.0$ mD. Permeability of the fracture domain is set as $k^f = 1$ Darcy. The lower transfer function leads to lower CO₂ saturation and a lower total mass fraction in the matrix. We also note that the CO₂ migrates further for a lower transfer function.

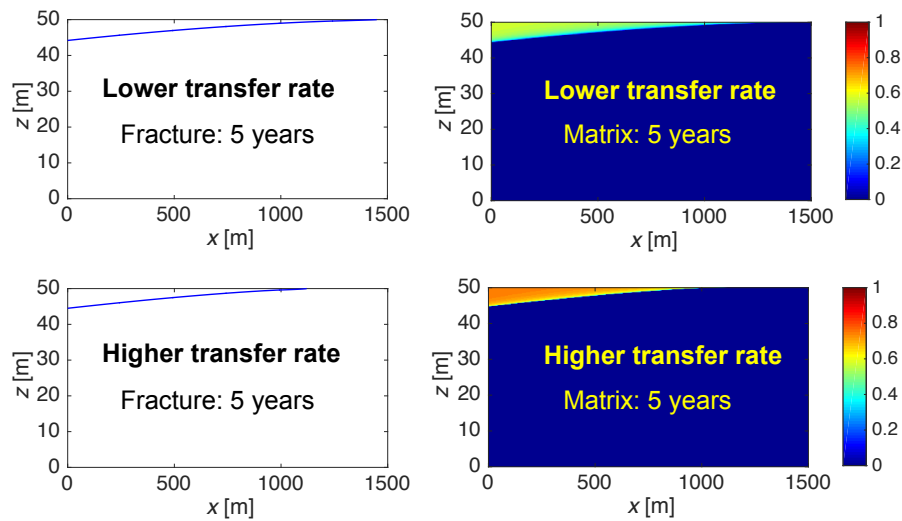


Figure 4: Simulation results of the CO₂ distributions from the VE dual-porosity model with a lower and a higher mass transfer rate between the fracture and the matrix.

5. Conclusions

In this paper, we have developed a dual-continuum vertically integrated modeling framework for CO₂ injection and migration in fractured geological formations. Fluid flow in the fracture domain is always modeled using a VE sharp interface model, while the matrix flow can be modeled with different approaches, which leads to different types of vertically integrated models. Preliminary results show that the VE sharp interface model is a good approximation for CO₂ migration in the fracture. By taking advantage of the dimension reduction from vertical integration, these models are much more computationally efficient compared to full multidimensional models. Different treatment of the matrix flow leads to a range of models with different levels of complexity, which provide useful modeling tools for analysis of CO₂ sequestration in fractured geological formations.

Acknowledgements

This material is based upon work supported by the Carbon Mitigation Initiative at Princeton University and by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) under Grant Number FE0023323. This project is managed and administered by Princeton University and funded by DOE/NETL and cost-sharing partners. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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