Multiscale Modeling of Carbon Dioxide Migration and Trapping in Fractured Reservoirs with Validation by Model Comparison and Real-Site Applications

Project Number DE-FE0023323

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U.S. Department of Energy

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Mastering the Subsurface Through Technology, Innovation and Collaboration:
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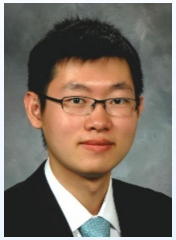
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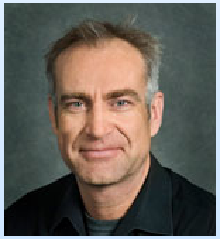
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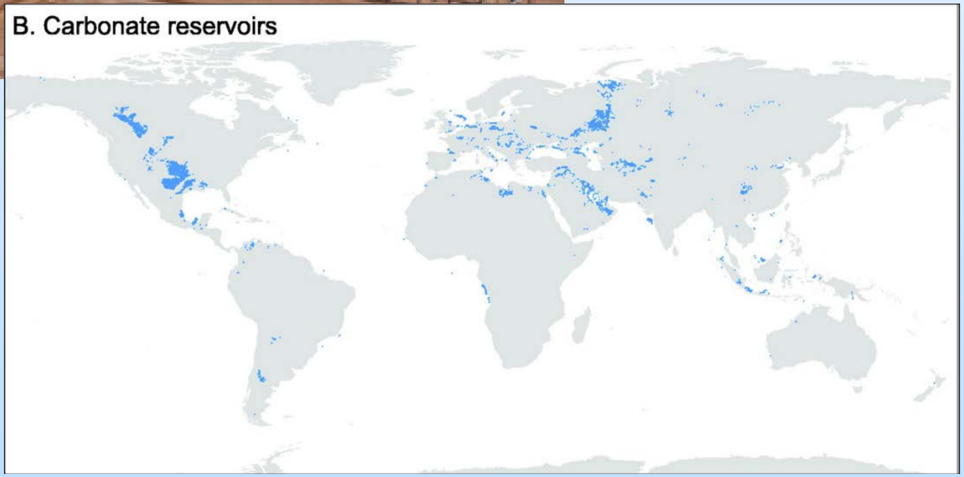
Presentation Outline

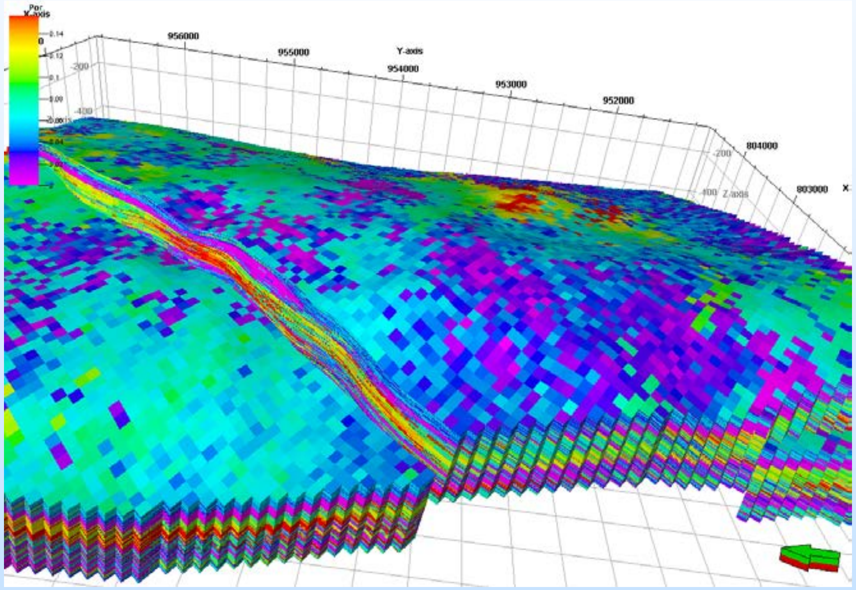
- Modeling approach
- Mass transfer models:
  - Diffusion
  - Gravity drainage
  - Spontaneous imbibition
- Vertically-integrated approach
- Key findings

Why fractured formations?

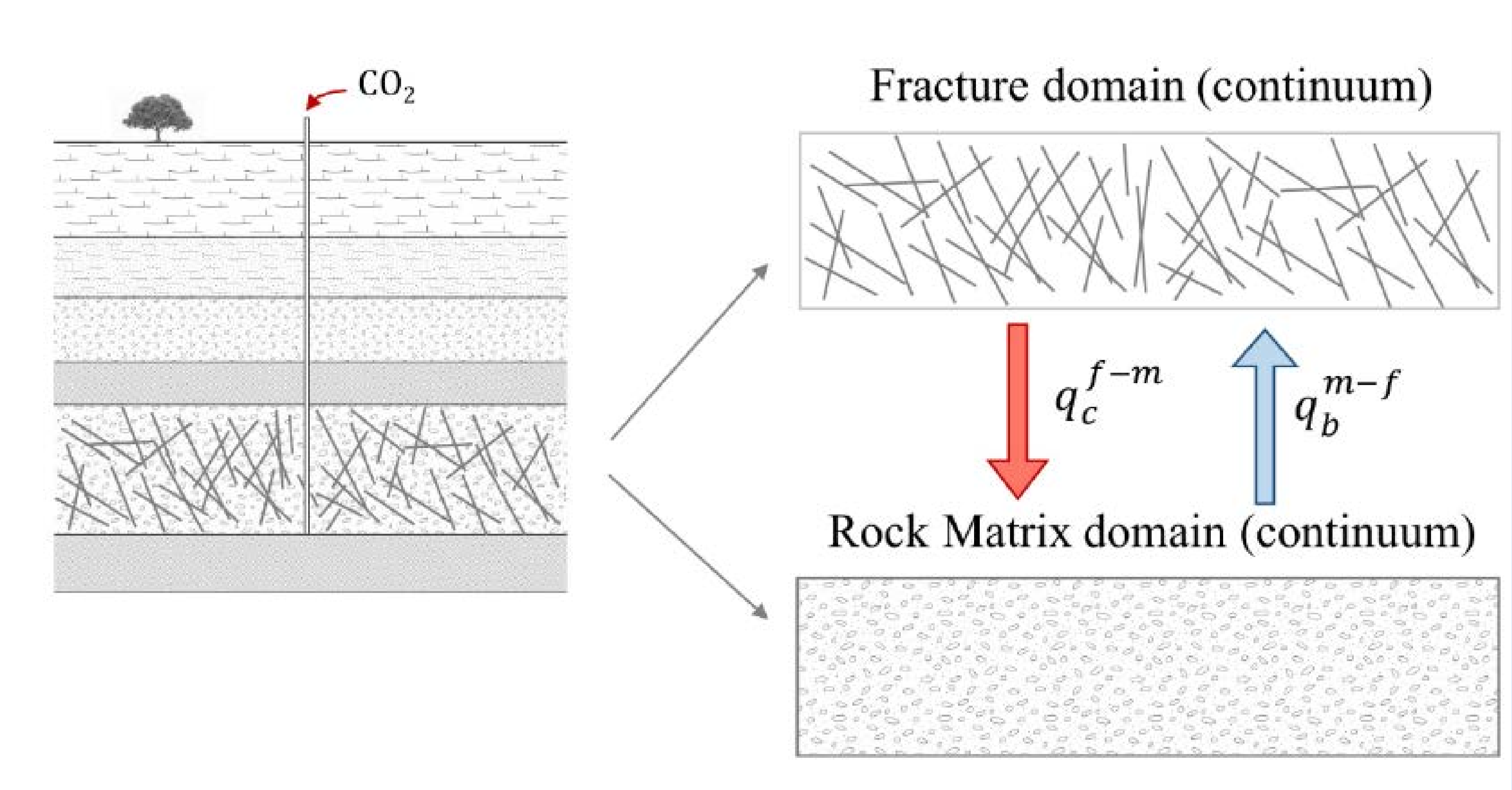


Ehrenberg & Nadeau (2005), AAPG Bulletin

What are the issues

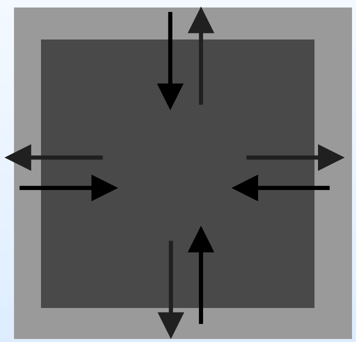


Dual domain approach

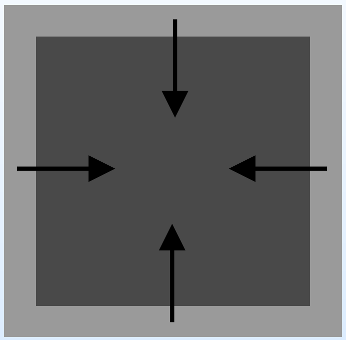


Fracture/Matrix Interaction

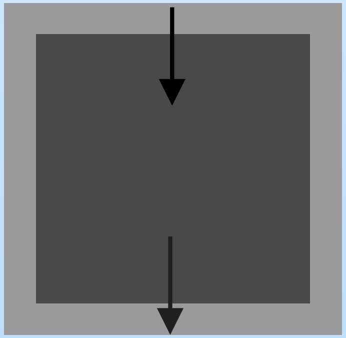
Spontaneous Imbibition



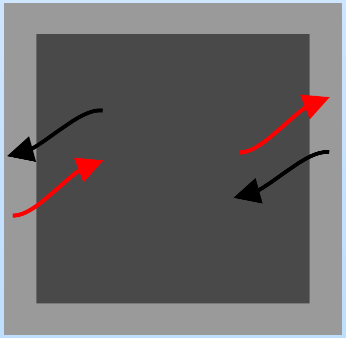
Fluid Compression



Gravity Displacement

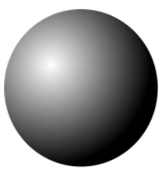
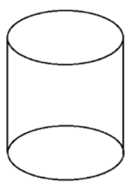
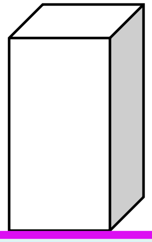
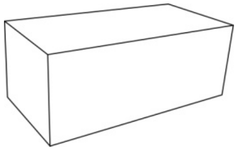
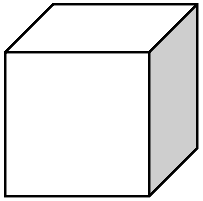


Molecular Diffusion



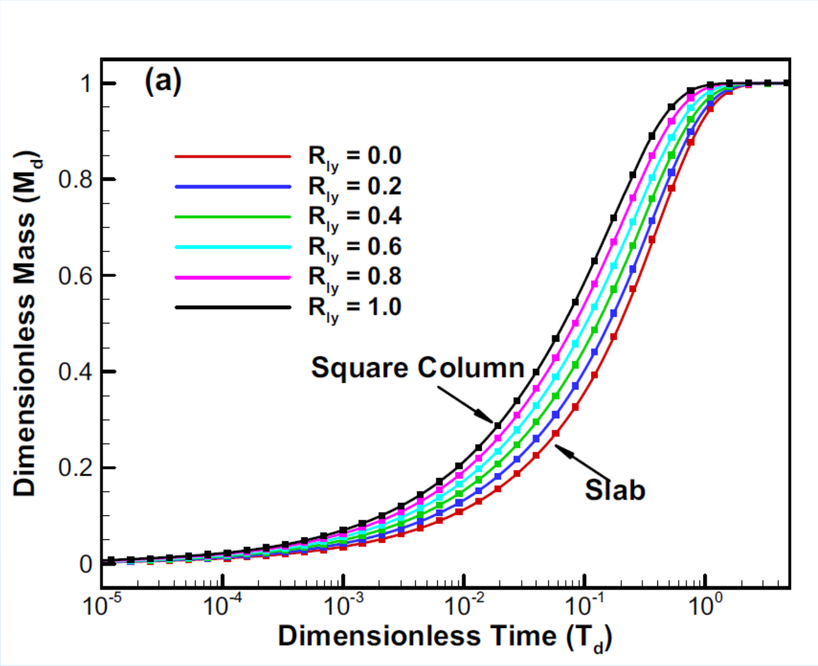
DIFFUSION

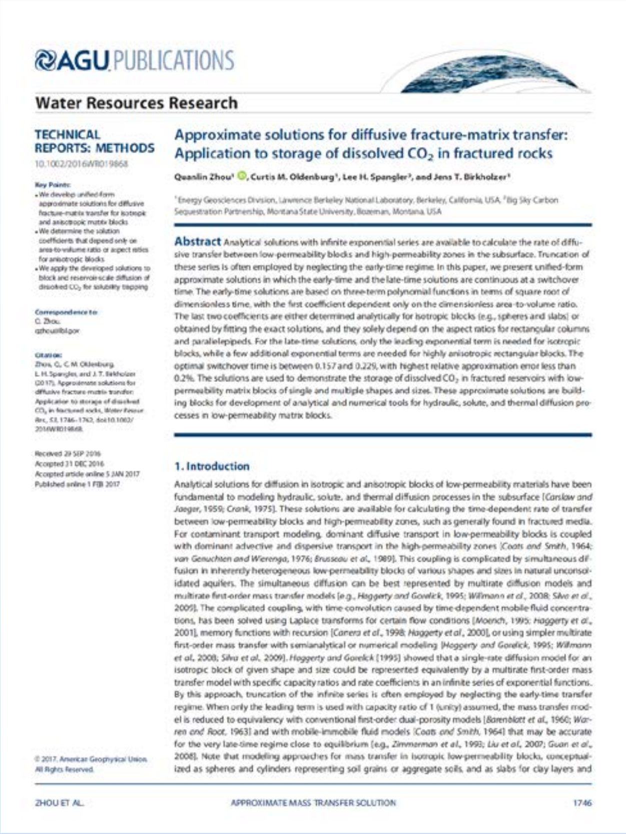
Analytic solutions

Sphere	Cylinder	Slab	Rectang. Column	Square Column	Rectang. Box	Cube
						

$$M_d = \begin{cases} a_1\sqrt{T_d} + a_2 T_d + a_3 (T_d)^{3/2} & T_d \leq T_{d0} \\ 1 - \sum_{j=1}^{N} b_{1j} \exp[-b_{2j} T_d], & T_d > T_{d0} \end{cases}$$

Accuracy





AGU PUBLICATIONS

Water Resources Research

TECHNICAL REPORTS: METHODS

10.1002/2016WR019868

Approximate solutions for diffusive fracture-matrix transfer: Application to storage of dissolved CO_2 in fractured rocks

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[1] Energy Geosciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA, [2] Big Sky Carbon Sequestration Partnership, Montana State University, Bozeman, Montana, USA

Key Points:

- We develop unified-form approximate solutions for diffusive fracture-matrix transfer for isotropic and anisotropic matrix blocks
- We determine the solution coefficients that depend only on area-to-volume ratio or aspect ratios for anisotropic blocks
- We apply the developed solutions to block and reservoir-scale diffusion of dissolved CO_2 for solubility trapping

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Zhou, Q., C. M. Oldenburg, L. H. Spangler, and J. T. Birkholzer (2017), Approximate solutions for diffusive fracture-matrix transfer: Application to storage of dissolved CO_2 in fractured rocks, *Water Resour. Res.*, 53, 1746–1762, doi:10.1002/2016WR019868.

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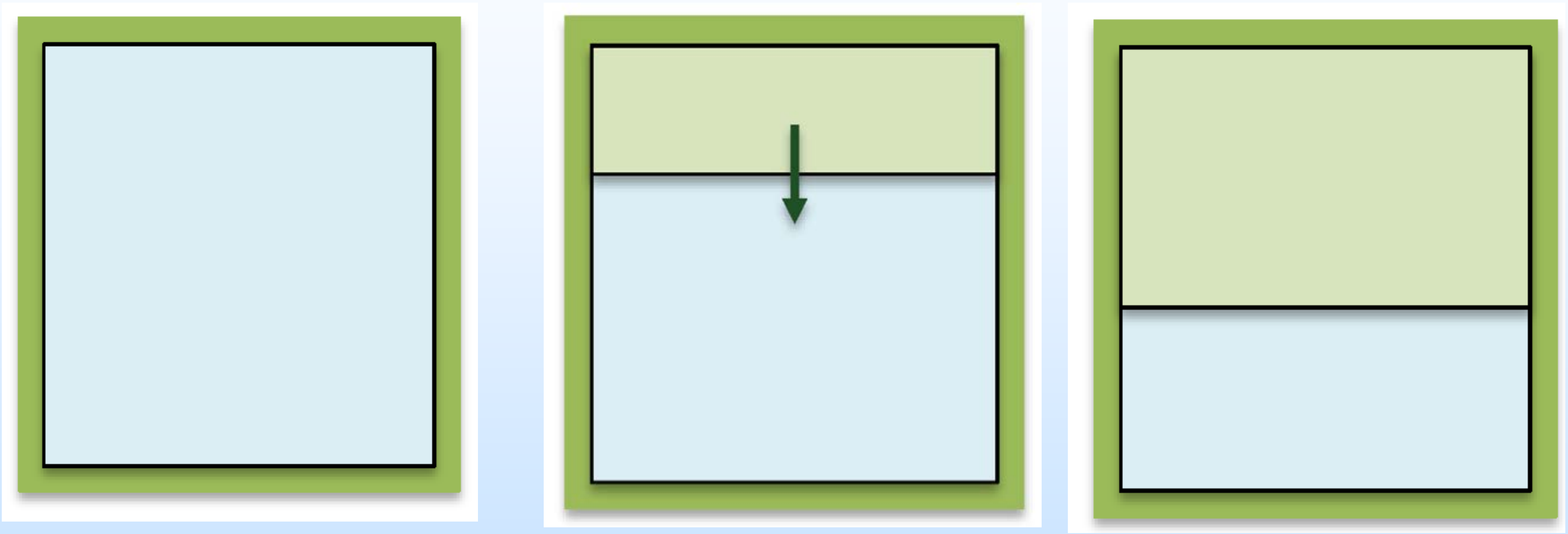
Abstract Analytical solutions with infinite exponential series are available to calculate the rate of diffusive transfer between low-permeability blocks and high-permeability zones in the subsurface. Truncation of these series is often employed by neglecting the early-time regime. In this paper, we present unified-form approximate solutions in which the early-time and the late-time solutions are continuous at a switchover time. The early-time solutions are based on three-term polynomial functions in terms of square root of dimensionless time, with the first coefficient dependent only on the dimensionless area-to-volume ratio. The last two coefficients are either determined analytically for isotropic blocks (e.g., spheres and slabs) or obtained by fitting the exact solutions, and they solely depend on the aspect ratios for rectangular columns and parallelepipeds. For the late-time solutions, only the leading exponential term is needed for isotropic blocks, while a few additional exponential terms are needed for highly anisotropic rectangular blocks. The optimal switchover time is between 0.157 and 0.229, with highest relative approximation error less than 0.2%. The solutions are used to demonstrate the storage of dissolved CO_2 in fractured reservoirs with low-permeability matrix blocks of single and multiple shapes and sizes. These approximate solutions are building blocks for development of analytical and numerical tools for hydraulic, solute, and thermal diffusion processes in low-permeability matrix blocks.

1. Introduction

Analytical solutions for diffusion in isotropic and anisotropic blocks of low-permeability materials have been fundamental to modeling hydraulic, solute, and thermal diffusion processes in the subsurface [*Carslaw and Jaeger*, 1959; *Crank*, 1975]. These solutions are available for calculating the time-dependent rate of transfer between low-permeability blocks and high-permeability zones, such as generally found in fractured media. For contaminant transport modeling, dominant diffusive transport in low-permeability blocks is coupled with dominant advective and dispersive transport in the high-permeability zones [*Coats and Smith*, 1964; *van Genuchten and Wierenga*, 1976; *Brusseau et al.*, 1989]. This coupling is complicated by simultaneous diffusion in inherently heterogeneous low-permeability blocks of various shapes and sizes in natural unconsolidated aquifers. The simultaneous diffusion can be best represented by multirate diffusion models and multirate first-order mass transfer models [e.g., *Haggerty and Gorelick*, 1995; *Willmann et al.*, 2008; *Silva et al.*, 2009]. The complicated coupling, with time-convolution caused by time-dependent mobile-fluid concentrations, has been solved using Laplace transforms for certain flow conditions [*Moench*, 1995; *Haggerty et al.*, 2001], memory functions with recursion [*Carrera et al.*, 1998; *Haggerty et al.*, 2000], or using simpler multirate first-order mass transfer with semianalytical or numerical modeling [*Haggerty and Gorelick*, 1995; *Willmann et al.*, 2008; *Silva et al.*, 2009]. *Haggerty and Gorelick* [1995] showed that a single-rate diffusion model for an isotropic block of given shape and size could be represented equivalently by a multirate first-order mass transfer model with specific capacity ratios and rate coefficients in an infinite series of exponential functions. By this approach, truncation of the infinite series is often employed by neglecting the early-time transfer regime. When only the leading term is used with capacity ratio of 1 (unity) assumed, the mass transfer model is reduced to equivalency with conventional first-order dual-porosity models [*Barenblatt et al.*, 1960; *Warren and Root*, 1963] and with mobile-immobile fluid models [*Coats and Smith*, 1964] that may be accurate for the very late-time regime close to equilibrium [e.g., *Zimmerman et al.*, 1993; *Liu et al.*, 2007; *Guan et al.*, 2008]. Note that modeling approaches for mass transfer in isotropic low-permeability blocks, conceptualized as spheres and cylinders representing soil grains or aggregate soils, and as slabs for clay layers and

GRAVITY DRAINAGE

Gravity drainage



Fractures filled with CO_2, matrix with brine

Buoyancy drives CO_2 into matrix

Capillary-gravity equilibrium

1D fractional flow

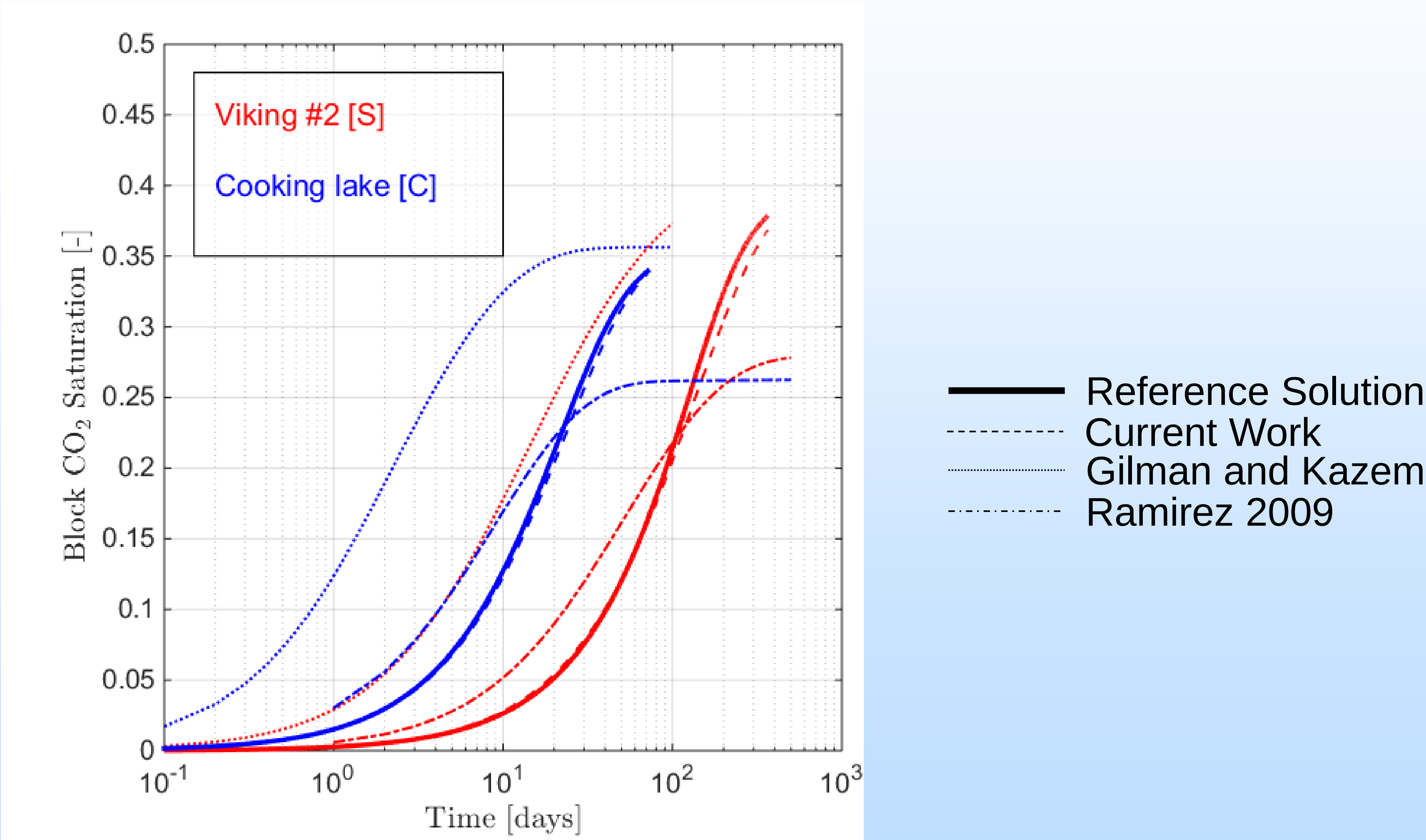
$$\phi \frac{\partial S_w}{\partial t} = -\frac{\partial}{\partial z}\left(f_w q_t + k f_w \lambda_n \Delta\rho g + k f_w \lambda_n \frac{\partial P_c}{\partial z} \right)$$

$$\frac{1}{\Delta t} \approx \frac{1}{\phi H}\frac{1}{\Delta S_w}\left\{ \overbrace{\bar{q}_t \cdot \max_{S_w}(f_w)}^{w_v} + \overbrace{k\Delta\rho g \cdot \max_{S_w}(f_w\lambda_n)}^{w_g} + \overbrace{k\frac{\Delta S_w}{H} \cdot \max_{S_w}\left(f_w\lambda_n \frac{dP_c}{dS_w} \right)}^{w_c} \right\}$$

$$\beta = \left(w_g + w_v + w_c \right)$$

$$T(S_{nm}, S_{nf}) = F(S_{nf})\beta(S_{nm} - S_n^{max})$$

Model comparison

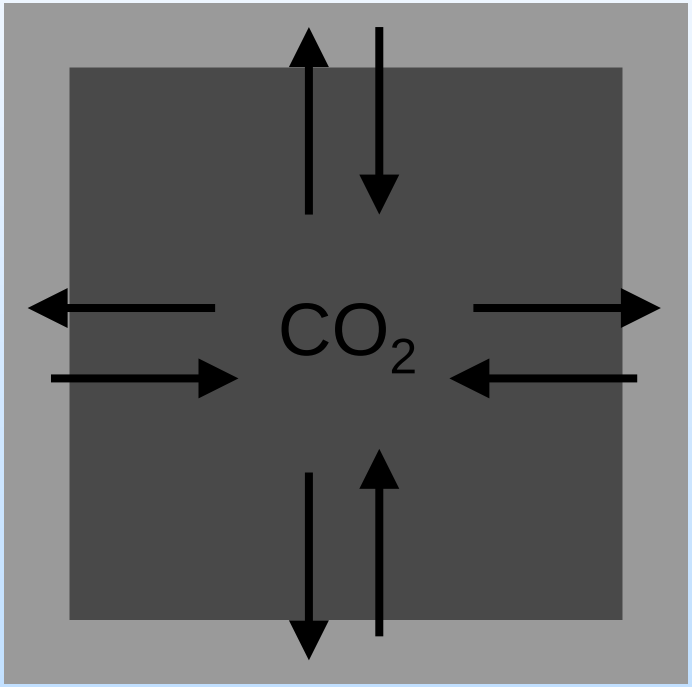


SPONTANEOUS IMBIBITION

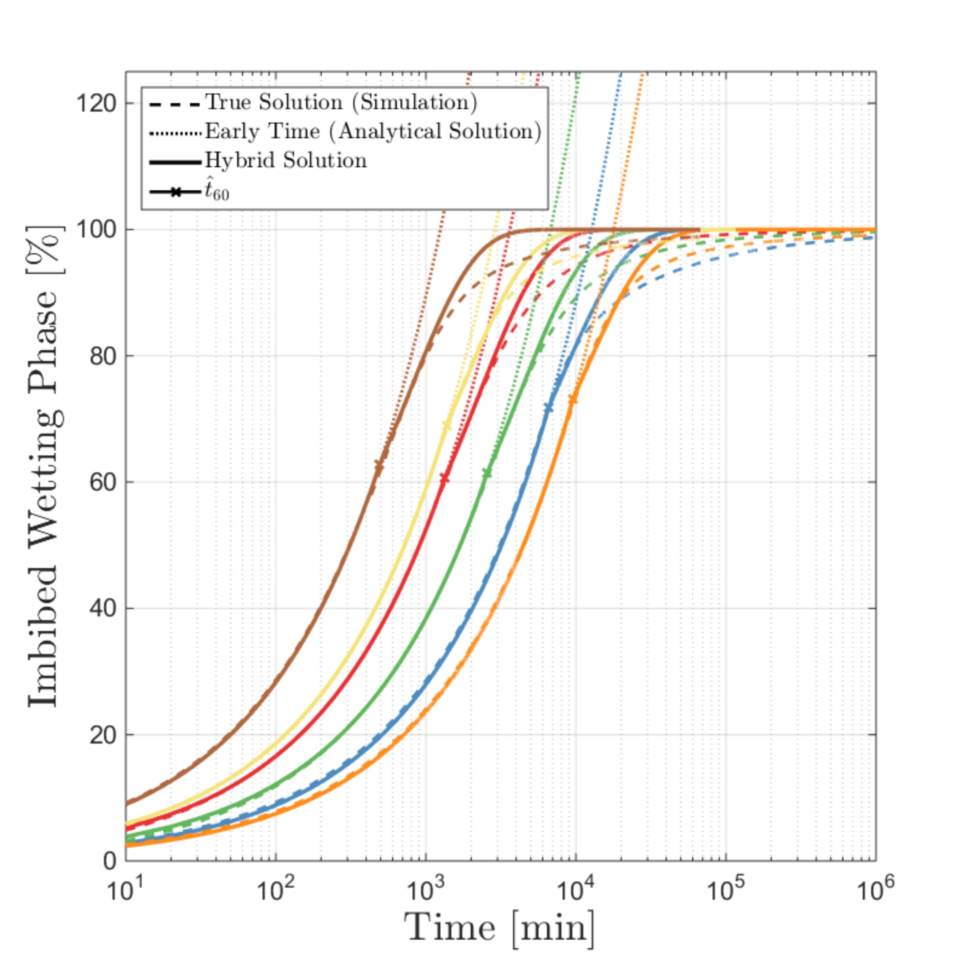
Spontaneous imbibition

Fracture filled with brine
Matrix filled with CO_2

Coffee cup filled with water
Sugar cube filled with air



Hybrid model



AGU PUBLICATIONS

Water Resources Research

RESEARCH ARTICLE

10.1002/2015WR018456

Accurate early-time and late-time modeling of countercurrent spontaneous imbibition

Rafael March[1], Florian Doster[1], and Sebastian Geiger[1]

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Key Points:

- New physically based model for spontaneous imbibition
- Model captures transition from early-time to late-time imbibition
- Model validated for different applications

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March, R., F. Doster, and S. Geiger (2016), Accurate early-time and late-time modeling of countercurrent spontaneous imbibition, *Water Resour. Res.*, 52, 6263–6276, doi:10.1002/2015WR018456.

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Abstract Spontaneous countercurrent imbibition into a finite porous medium is an important physical mechanism for many applications, included but not limited to irrigation, CO_2 storage, and oil recovery. Symmetry considerations that are often valid in fractured porous media allow us to study the process in a one-dimensional domain. In 1-D, for incompressible fluids and homogeneous rocks, the onset of imbibition can be captured by self-similar solutions and the imbibed volume scales with $\sqrt{t}$. At later times, the imbibition rate decreases and the finite size of the medium has to be taken into account. This requires numerical solutions. Here we present a new approach to approximate the whole imbibition process semianalytically. The onset is captured by a semianalytical solution. We also provide an a priori estimate of the time until which the imbibed volume scales with $\sqrt{t}$. This time is significantly longer than the time it takes until the imbibition front reaches the model boundary. The remainder of the imbibition process is obtained from a self-similarity solution. We test our approach against numerical solutions that employ parametrizations relevant for oil recovery and CO_2 sequestration. We show that this concept improves common first-order approaches that heavily underestimate early-time behavior and note that it can be readily included into dual-porosity models.

1. Introduction

The spontaneous invasion of a wetting phase into a porous medium due to capillary forces is a remarkable physical phenomenon relevant to a wide range of geological and engineering applications. Perhaps most importantly, spontaneous imbibition (SI) is one of the main mechanisms of fluid exchange between fractures and matrix in fractured geological formations. Hence, understanding SI is of importance to optimize hydrocarbon recovery [*Morrow and Mason*, 2001; *Mason and Morrow*, 2013], model water injection into geothermal reservoirs [*Li and Horne*, 2009], understand the imbibition of brine into CO_2 saturated rocks in geological storage of carbon dioxide [*Nordbotten and Celia*, 2012], or analyze the migration of fracturing fluids in shale formations [*Birdsell et al.*, 2015; *Dehghanpour et al.*, 2013].

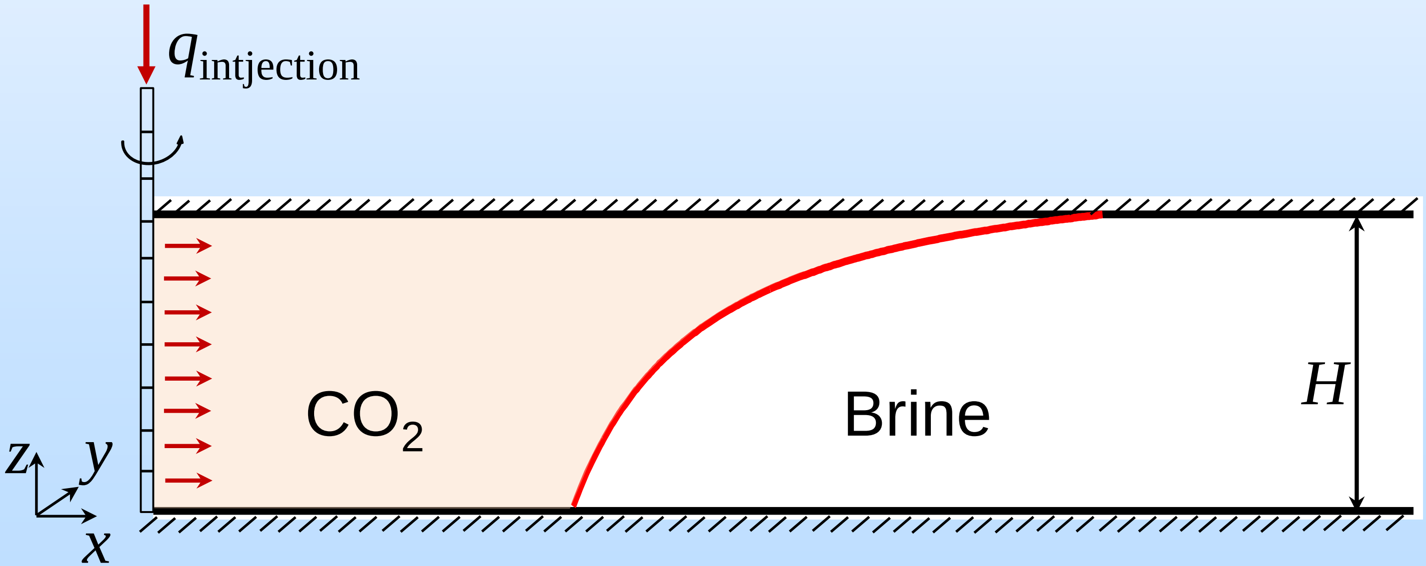
Countercurrent spontaneous imbibition is mathematically described by a nonlinear diffusion equation. Finding analytical solutions that are valid at early and late times has been an open challenge for many years. At early time, that is, before the advance of the wetting phase front is influenced by a no-flow boundary condition, the cumulative imbibed volume scales with $\sqrt{t}$ [*Lucas*, 1918; *Washburn*, 1921]. The late-time behavior, on the other hand, is characterized by a decrease in the imbibition rate. It is usually presumed to follow approximately an exponential expression of the form $V/V_\infty = 1 - e^{-\lambda t}$ [*Aronofsky et al.*, 1958], where λ describes the rate of the transfer process. Models for this parameter have been proposed over the last century [*Washburn*, 1921; *Li and Horne*, 2006; *Zhou et al.*, 2002; *Ma et al.*, 1997; *Mattax and Kyte*, 1962; *Tavassoli et al.*, 2005], but only recently a general scaling group based on the analytical solution for the countercurrent spontaneous imbibition in semi-infinite domain was developed [*Schmid and Geiger*, 2012, 2013]. This group properly includes the effects of rock wettability, viscosity ratio, and other physical parameters, such as arbitrary capillary pressure and relative permeability curves, and provides a good agreement with a large body of experimental data of spontaneous imbibition.

In the context of modeling and simulation of fractured reservoirs, dual-porosity models provide a framework for simulation of such geological formations by considering the fracture network as a second porous medium/continuum that is superposed to the matrix rock [*Warren and Root*, 1963]. The fluid interchange between the two continua is modeled by means of a transfer-rate function. In this sense, the exponential

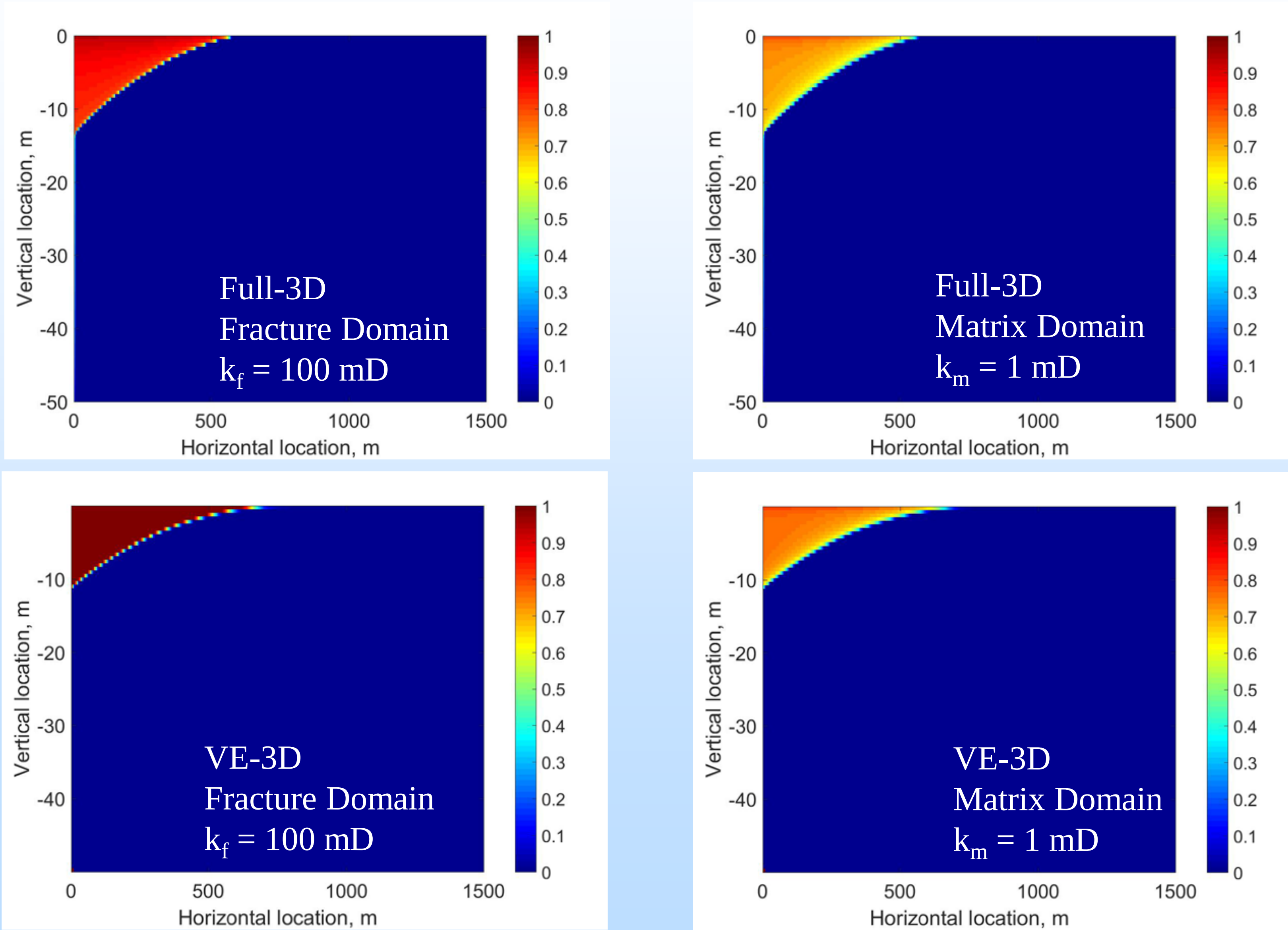
SIMPLIFIED MODEL

Simplified models

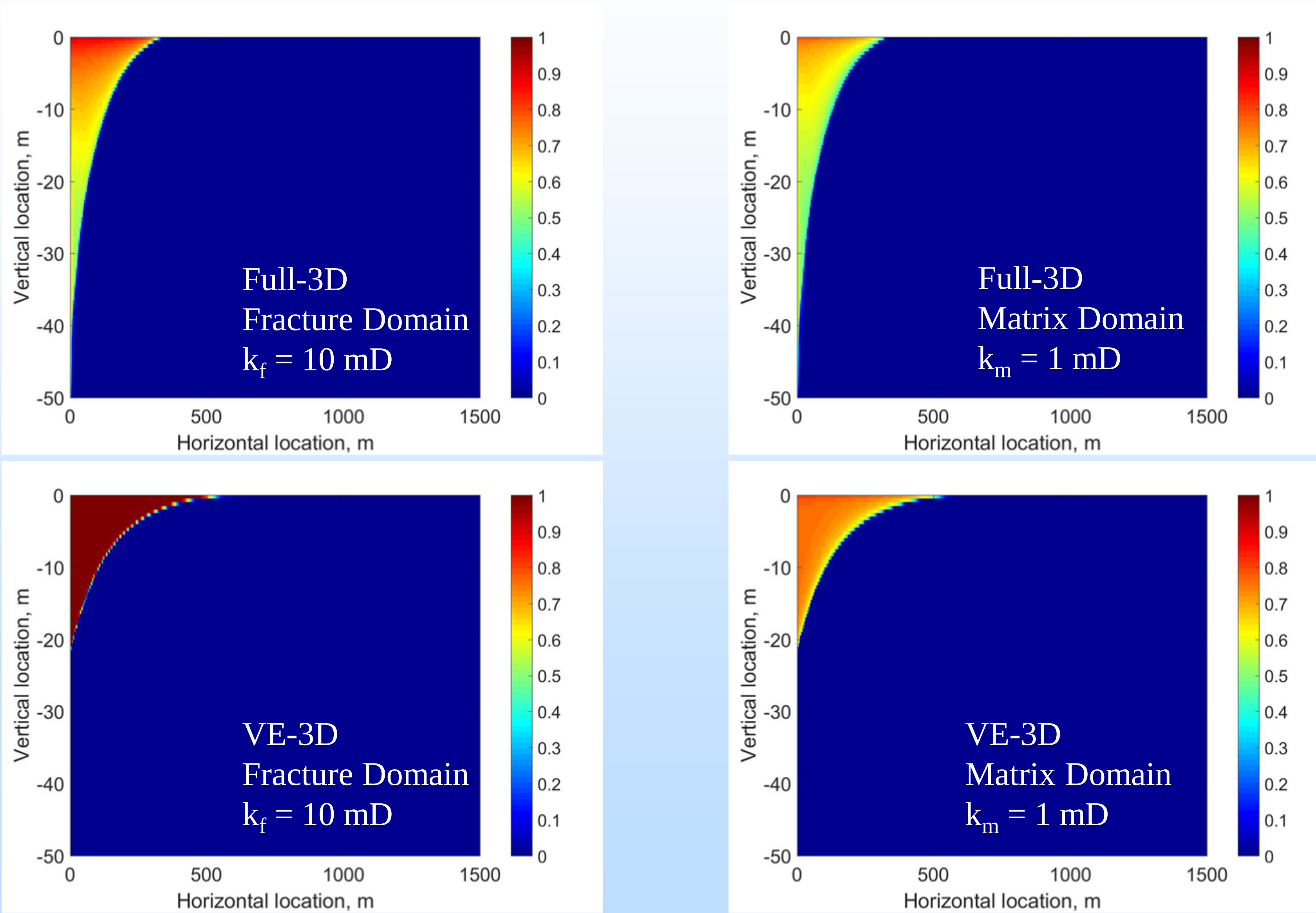
- Large spatial domains
- High uncertainty of fracture parameters
- High permeability of fractures



VE results (100 mD)



VE results (10 mD)



Key findings

- We can use relatively simple deterministic models to describe mass transfer based on:
  - Diffusion
  - Gravity drainage
  - Spontaneous imbibition
- Vertically-integrated models seem to be applicable

Accomplishments to Date

- Development of transfer function for dual-porosity model for both spontaneous imbibition and gravity drainage
- Implemented and validated single- and two-phase dual-porosity modules and a hysteresis module for MRST
- Updated TOUGH2/ECO2N simulator for better performance for CO_2 storage in fractured media simulations

Accomplishments to Date

- Investigated the impact of matrix block connectivity on CO_2 storage capacity
- Developed analytic solutions for CO_2 storage due to diffusion of dissolved CO_2
- Developed and implemented a vertically-integrated dual-porosity model
- Investigated development of vertically-integrated dual-permeability model

Lessons learned

- More complex is not necessarily better
- Vocabulary matters

Synergy opportunities

- The modeling approaches developed in this project should be useful to other projects studying carbon sequestration in fractured formations

Future Plans

- Continue development of vertically-integrated dual-porosity and dual-permeability models
- Continue to investigate the impact of fracture and matrix block parameters on CO_2 storage capacity
- Apply newly developed modeling approaches to In Salah site

THANK YOU!

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Appendix

Benefit to the Program

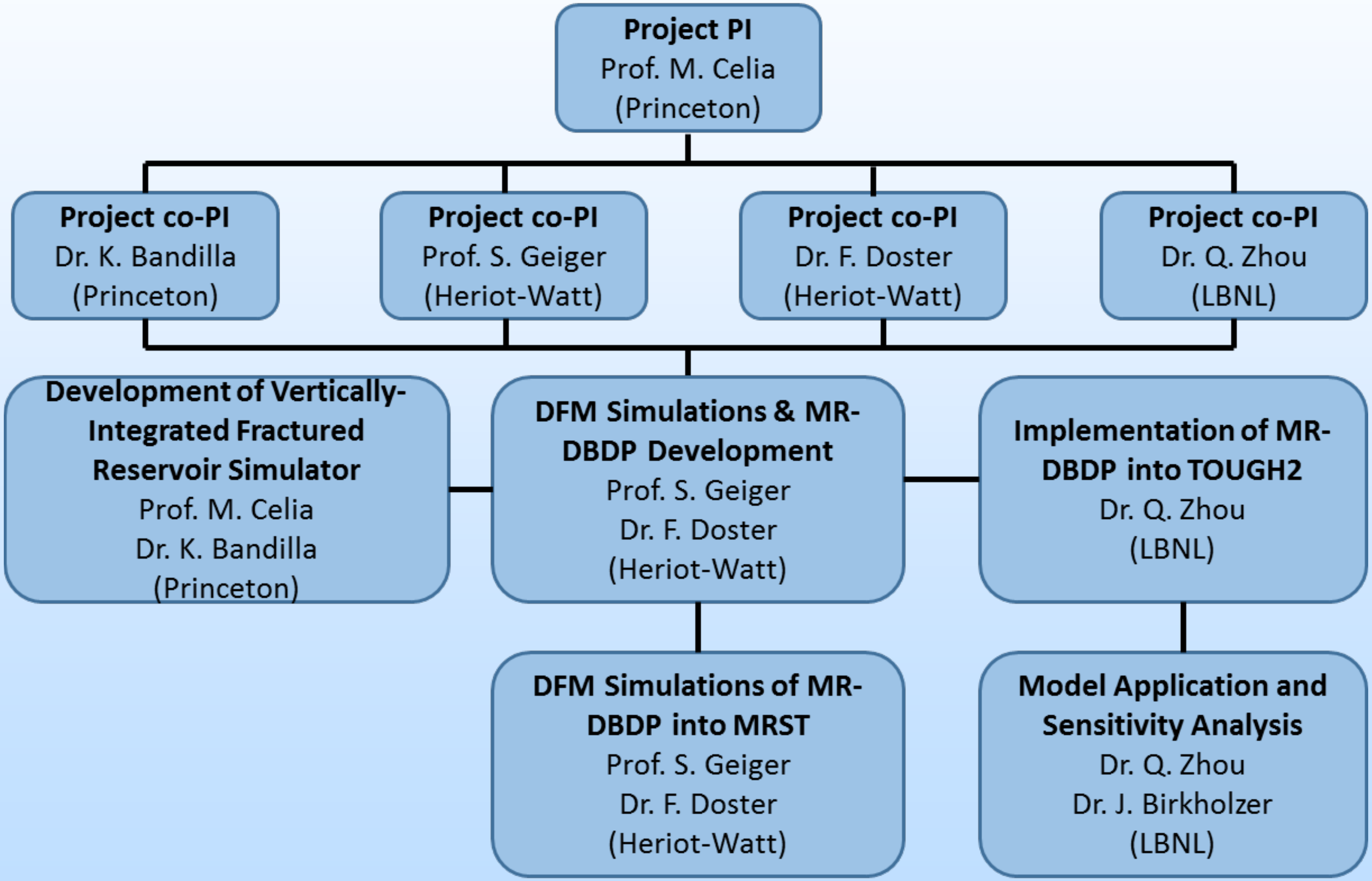
- Goal: Develop new capabilities for carbon sequestration modeling in fractured reservoirs through improvements in the representation of fracture-matrix flow interactions.

- Support industry's ability to predict CO_2 storage capacity in geologic formations to within ±30 percent.

Project Objectives

- Develop new models for interactions of fracture and matrix flow
- Incorporate those models into reservoir-scale simulators
- Conduct sensitivity analyses of trapping efficiency and storage capacity using new model
- Apply new model to In Salah site

Organization Chart



Gantt Chart

light grey: accomplished; dark grey: planned; MS: mile stone

Fiscal Year	BP 1				BP 2						BP 3	
Quarter	1	2	3	4	1	2	3	4	5	6	3	4
Task 1: Project Management, Planning and Reporting												
Subtask 1.1: Updated Project Management Plan	MS											
Subtask 1.2: Project Planning and Reporting	MS											
Task 2.0: Detailed DFM modeling of CO2 and brine				MS								
Task 3.0: Development of MR-DBDP model with analytic transfer function						MS						
Task 4.0: Development of new simulator capabilities												
Subtask 4.1: Development of vertically integrated simulator					MS					MS		
Subtask 4.2: incorporate new MR-DBDP into MRST simulator												MS
Subtask 4.3: incorporate new MR-DBDP into TOUGH2									MS			
Task 5.0: Model demonstration and sensitivity analysis												
Subtask 5.1: Investigation of driving forces												
Subtask 5.2: Sensitivity Analysis								MS				
Subtask 5.3: Storage and trapping in heterogeneous reservoir										MS		
Subtask 5.4: Investigation of injection scenarios												
Task 6.0: Simulator application to In Salah												
Subtask 6.1: Site-specific model development										MS		
Subtask 6.2: Migration and Trapping modeling										MS		
Subtask 6.3: Sensitivity analysis												MS

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