Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate

Project Number DE-FE0009563

Karl Bandilla

Princeton University

U.S. Department of Energy

National Energy Technology Laboratory

Mastering the Subsurface Through Technology, Innovation and Collaboration:
Carbon Storage and Oil and Natural Gas Technologies Review Meeting

August 16-18, 2016

Presentation Outline

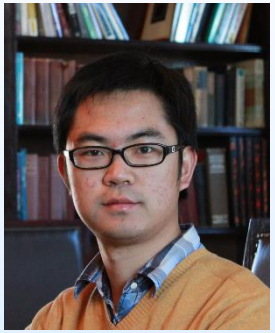
- Project Benefits, Goals and Objectives
- Project overview
- Accomplishments
- Summary

Project participants

Princeton University

Michael Celia

Karl Bandilla



Bo Guo

Lawrence Berkeley National Laboratory

Jens Birkholzer

Abdullah Cihan

Benefit to the Program

- Goal: Develop a suite of models, across a broad spectrum of complexity, and determine when simplified models are appropriate for CO_2 sequestration modeling.
- Develop Best Practice Manuals for monitoring, verification, accounting, and assessment; site screening, selection and initial characterization; public outreach; well management activities; and risk analysis and simulation.

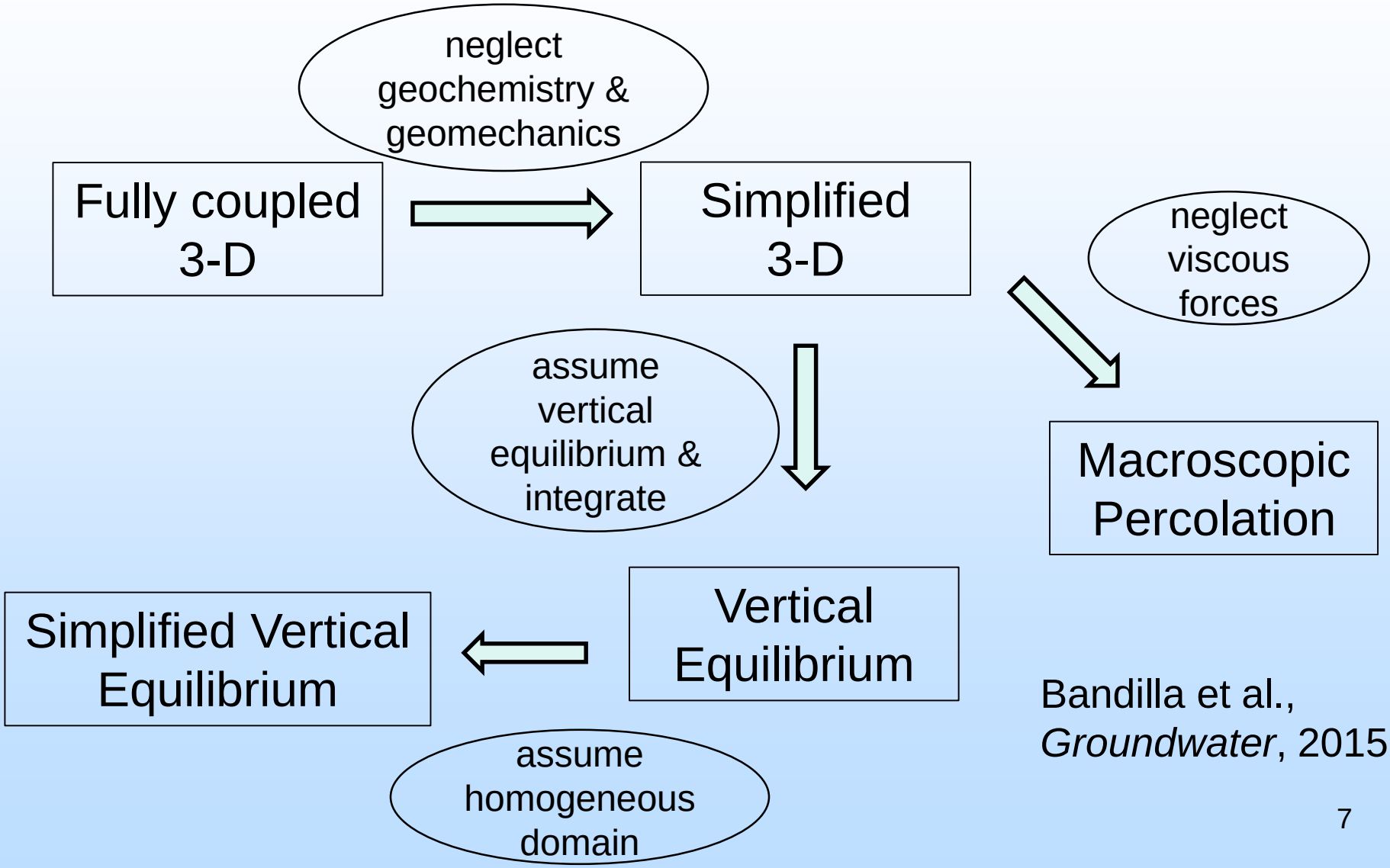
Project Objectives

- Assemble a suite of models across the range of complexity
- Compare the performance of models of different complexity when applied to actual sites
  - forward modeling
  - optimization
- Develop a set of practical criteria that can guide the choice of model complexity

Project Overview

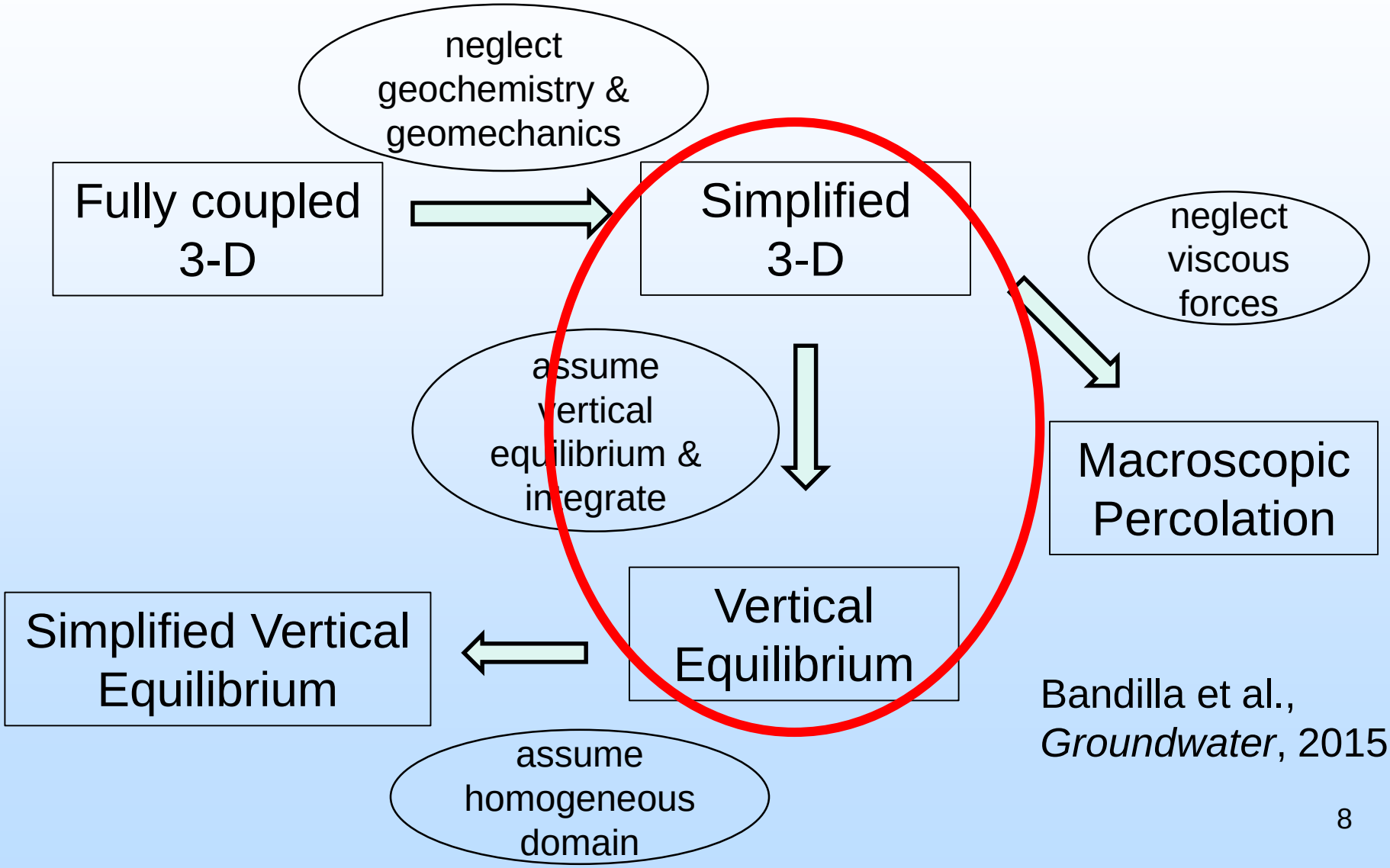
- Spectrum of model complexity
- Vertically-integrated models
  - vertical heterogeneity
  - dynamic reconstruction
- Model complexity guidelines
- Model optimization

Model Complexity



Bandilla et al., *Groundwater*, 2015

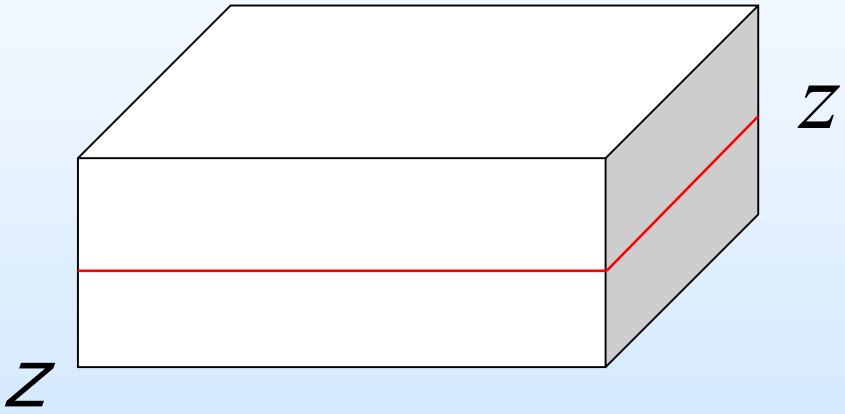
Model Complexity



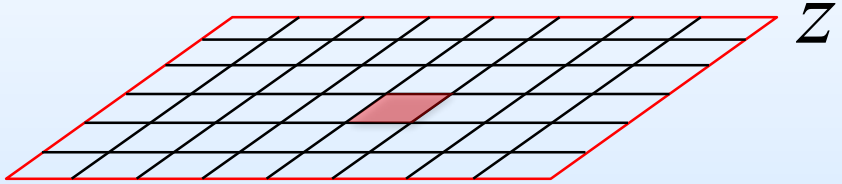
Bandilla et al., *Groundwater*, 2015

Vertically-integrated models

Full multi-dimensional system



Vertically-integrated system

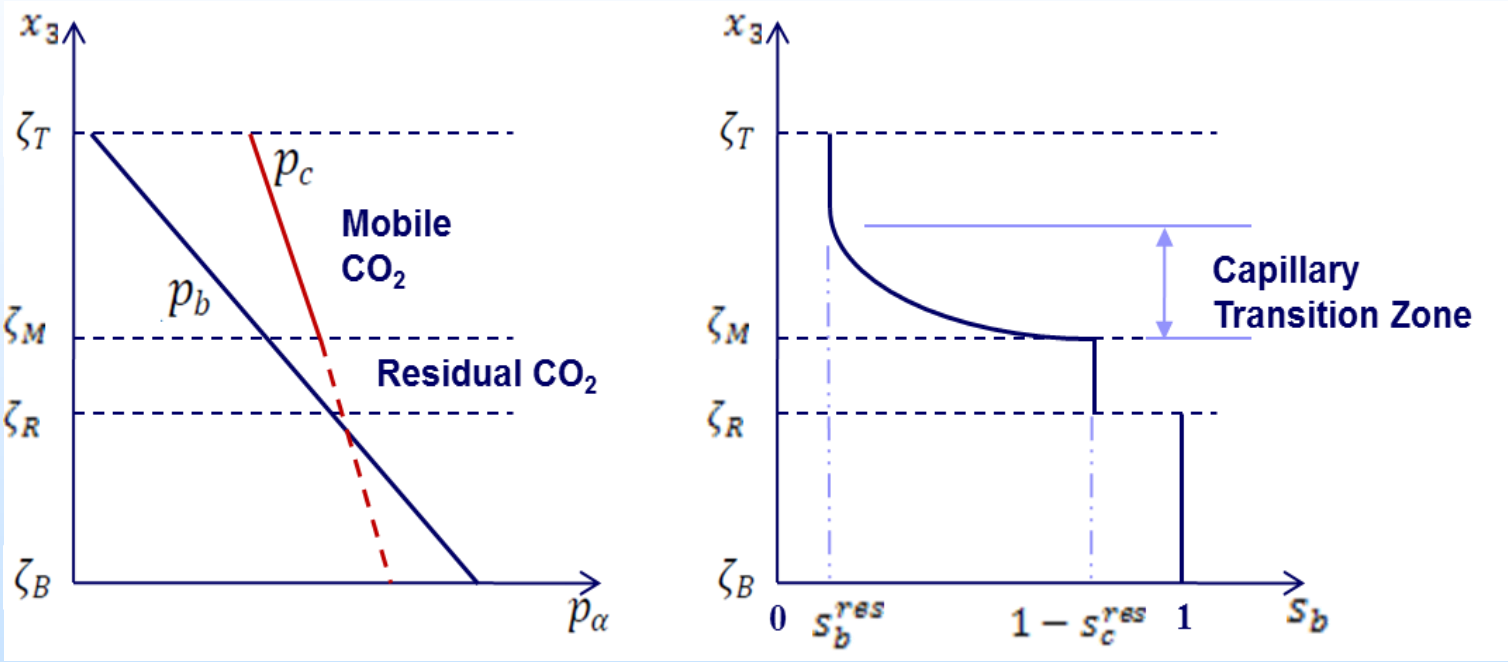


$$\Phi \frac{\partial(\rho_\alpha S_\alpha)}{\partial t} + \nabla_{||} \cdot (\rho_\alpha \mathbf{U}_\alpha) = Q_\alpha$$

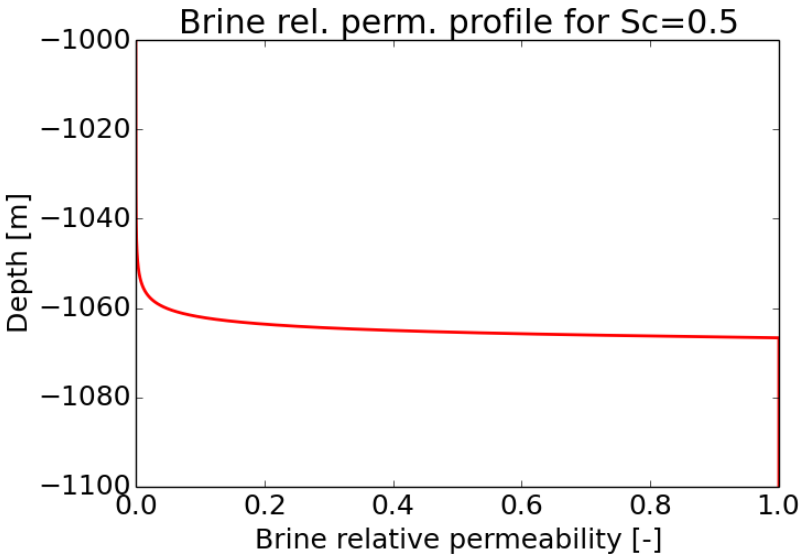
$$\mathbf{U}_\alpha = -\mathbf{K}\Lambda_\alpha(s_\alpha) \cdot (\nabla_{||} P_\alpha - \rho_\alpha \mathbf{G})$$

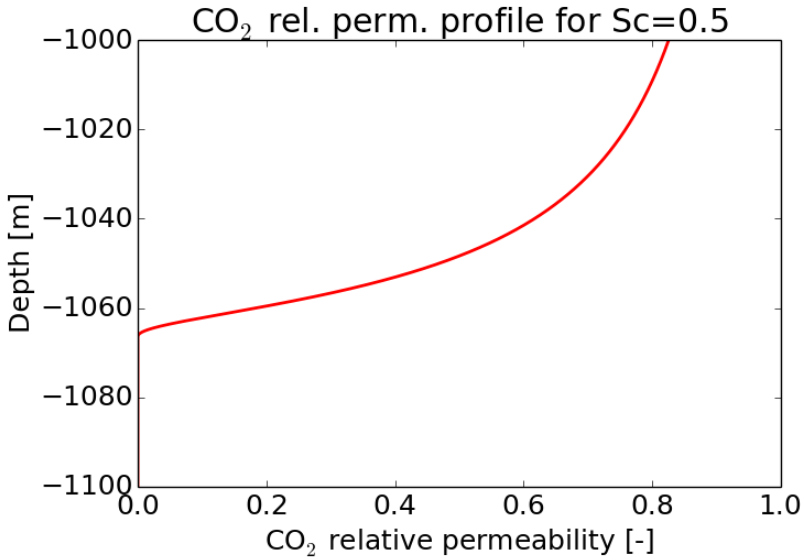
VERTICAL EQUILIBRIUM RECONSTRUCTION

Vertical Equilibrium

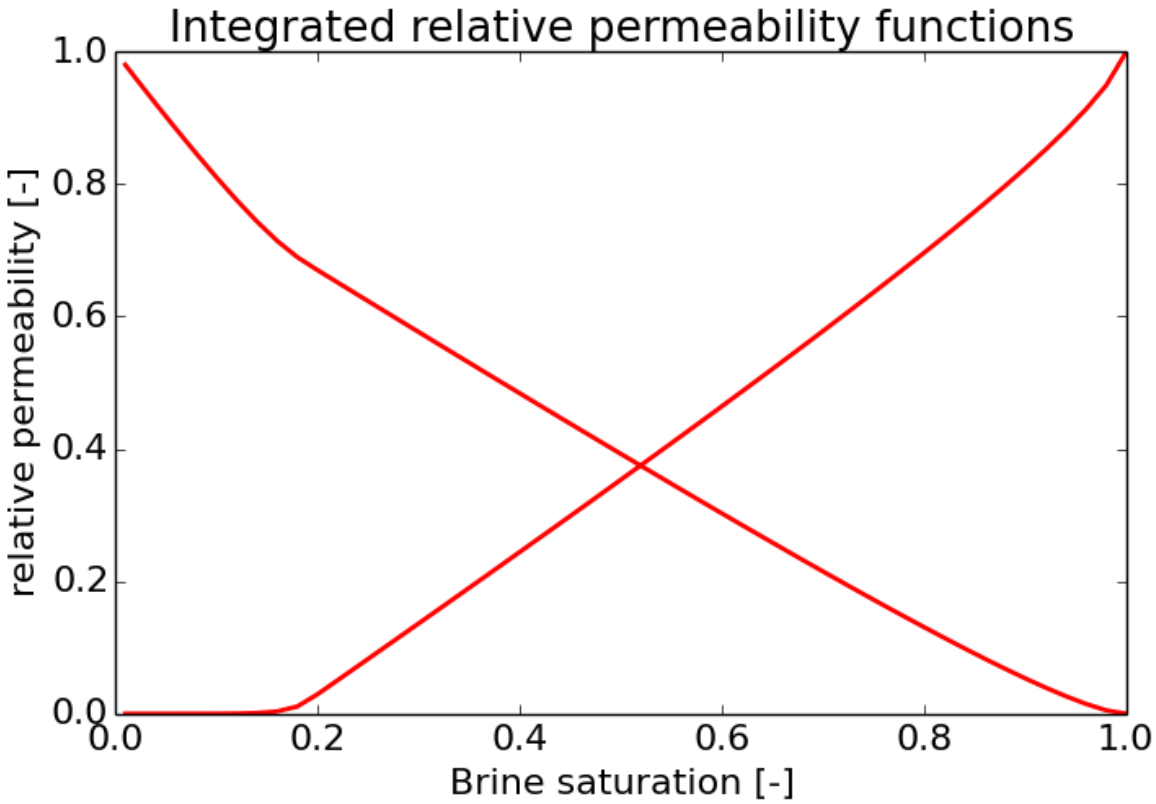


Rel perm profiles

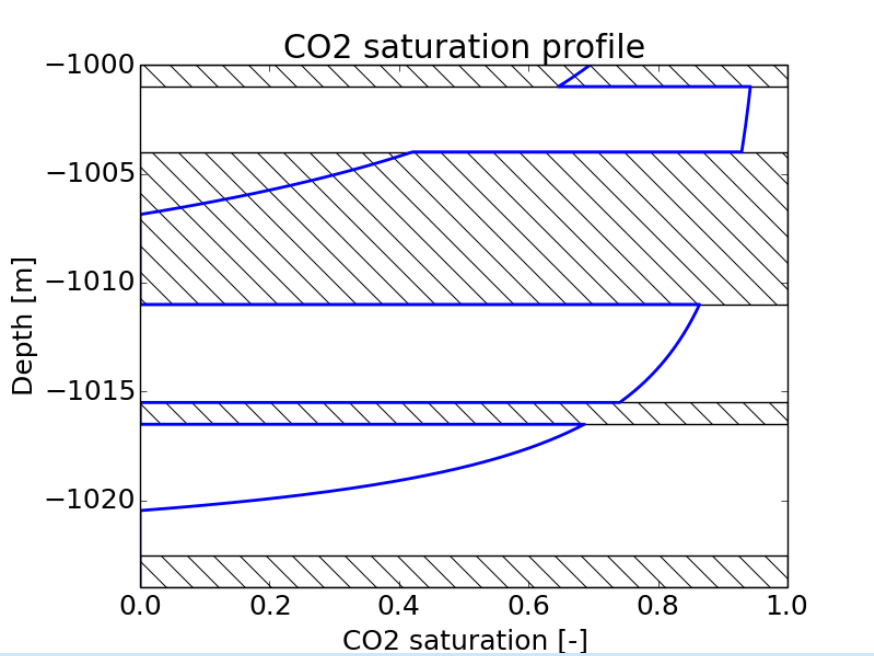


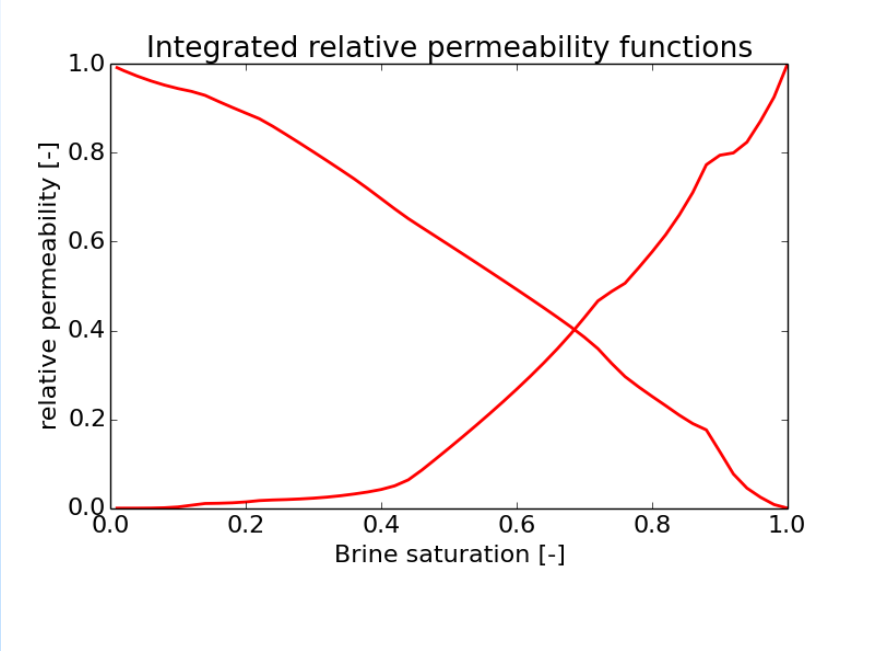


Integrated rel perms



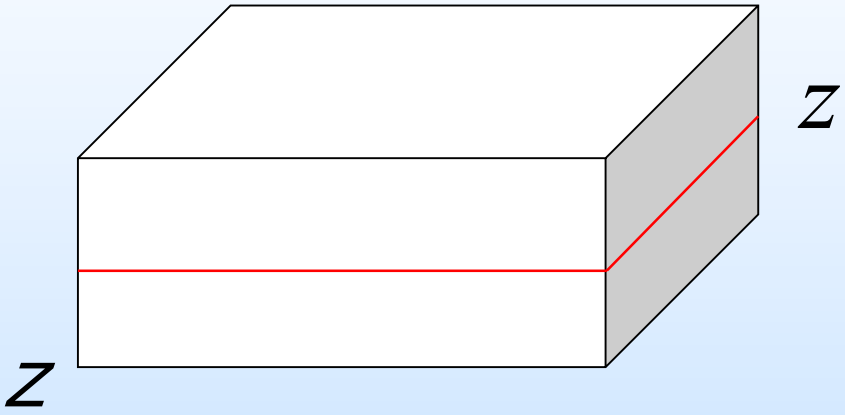
VE with heterogeneity





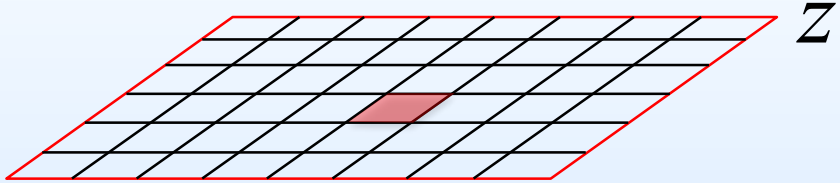
DYNAMIC VERTICAL RECONSTRUCTION

Dynamic reconstruction

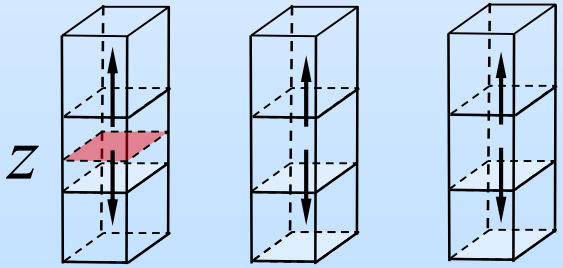


Full multi-dimensional system

Coarse Scale

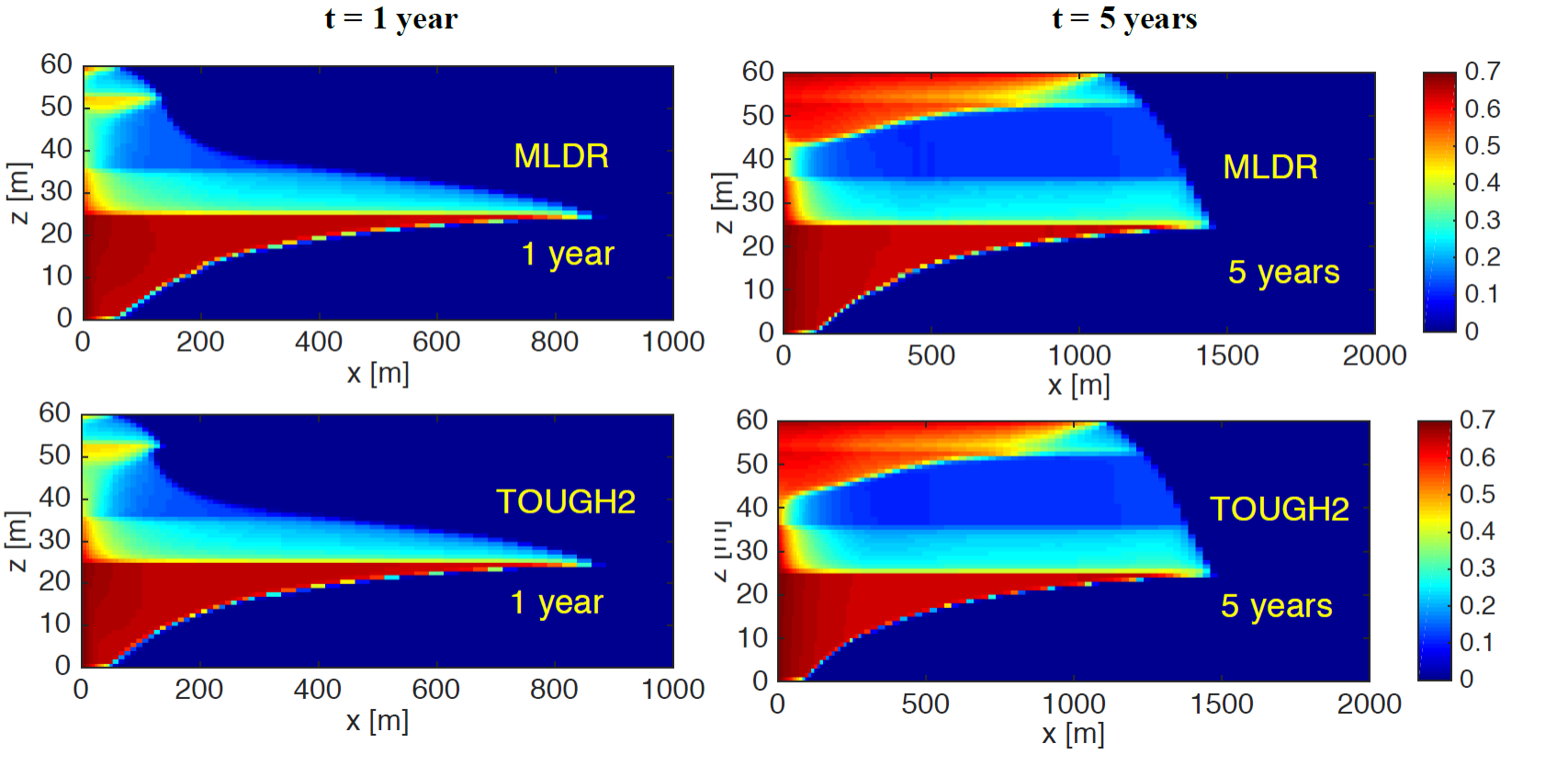


Fine Scale



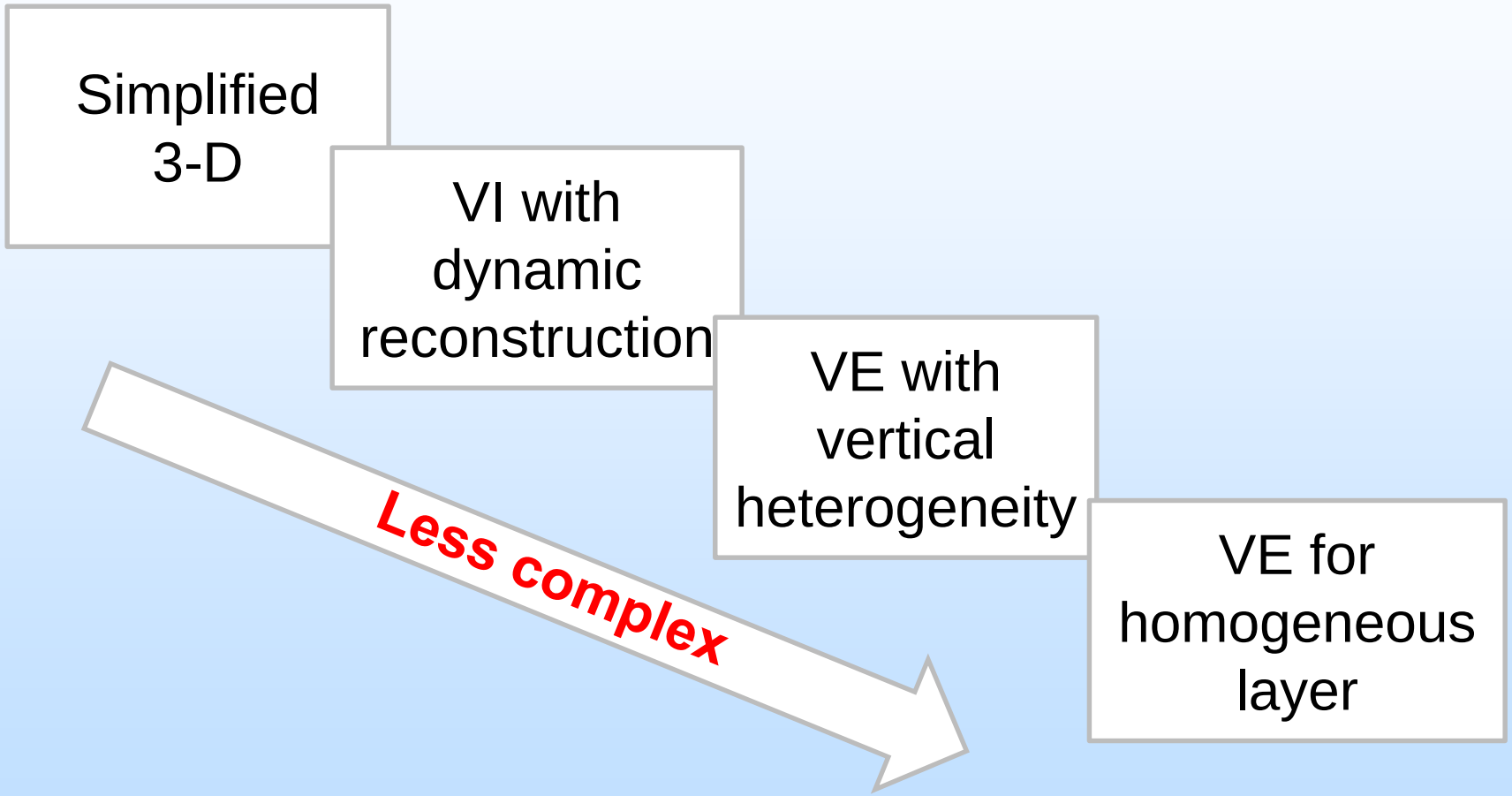
Guo et al., *WRR*, 2014

Example results



Guo et al., *WRR*, 2016

New complexity spectrum



Applicability

Semi-analytic VE

Spatial heterogeneity, capillary transition zone

numerical VE

Vertical permeability < 100mD, partial injection

Dynamic reconstruction

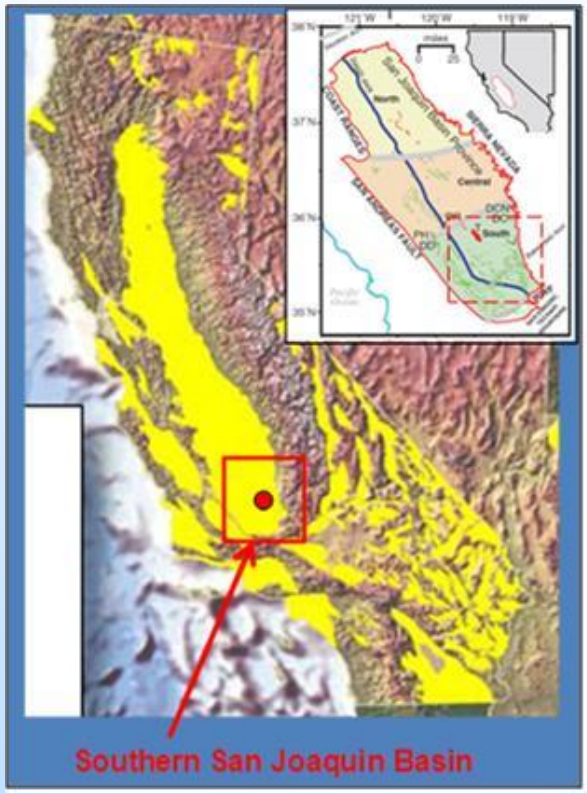
Complex vertical and horizontal heterogeneity, near well

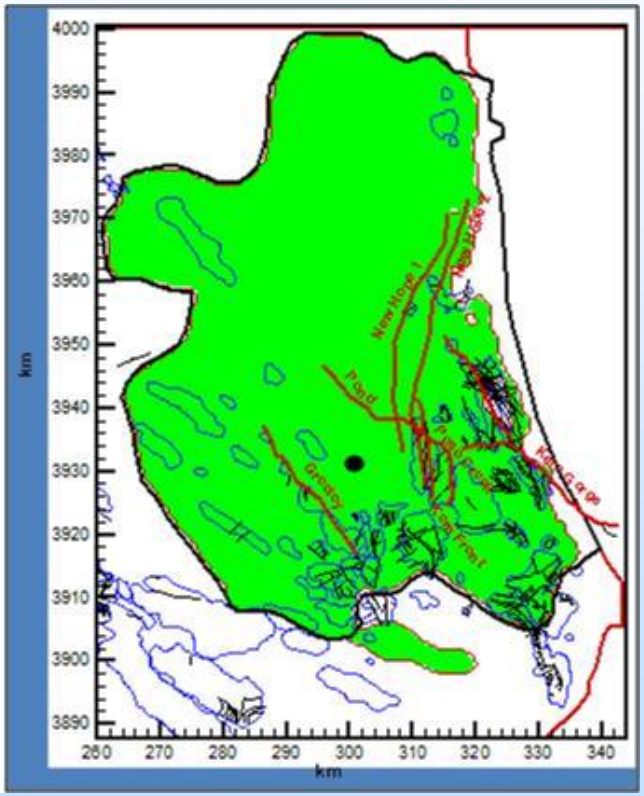
Simplified 3D

Strong feedback to flow properties

Multiphysics 3D

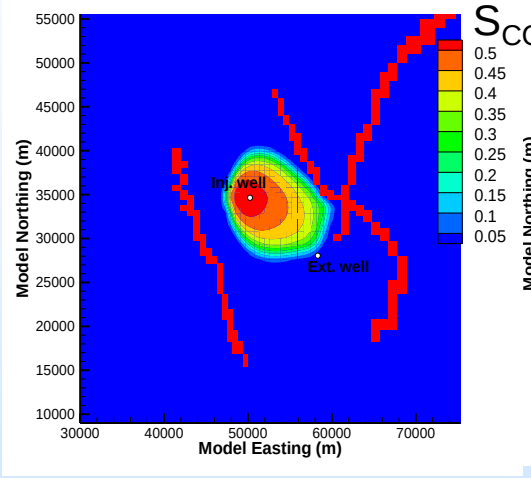
Optimization: Kimberlina



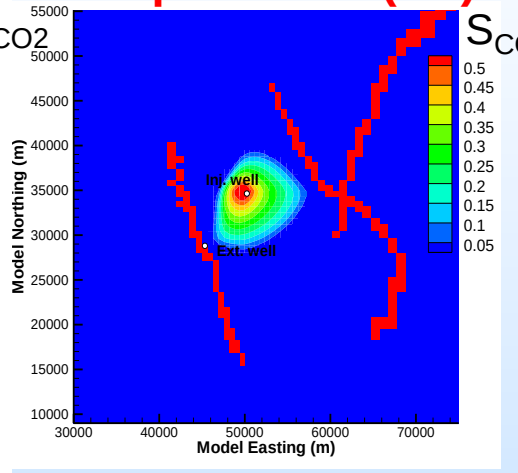


Optimization: results

Two-phase Flow in 3D

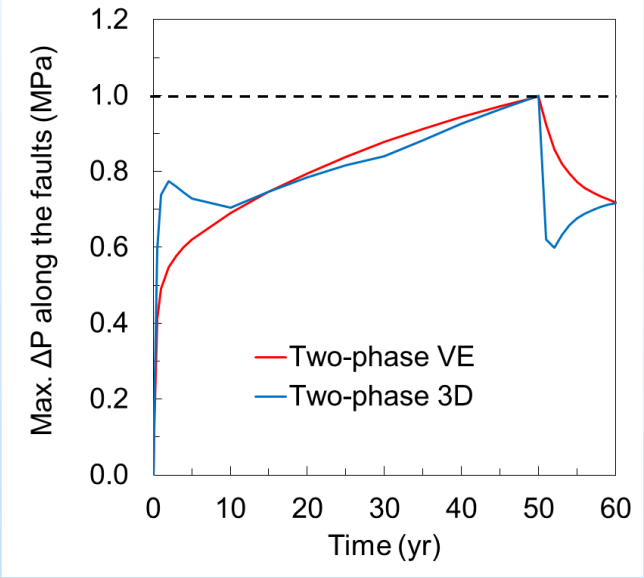


Two-phase Vertical Equilibrium (VE)



	Two phase Flow 3D	Two-phase Vertical Equilibrium
Easting ext. well (m)	45333	58240
Northing ext. well (m)	28656	28205
Optimal ext. rate (Mt/yr) for ΔP_{max}=1 MPa	4.5	5.0
Injection rate (Mt/yr)	5.0	5.0

Inj. rate= 5 Mt/yr



Summary

- Vertically-integrated model with dynamic reconstruction offers intermediate complexity between simplified 3D and vertical equilibrium
- Vertical heterogeneity can be included in vertical-equilibrium models
- Vertical-equilibrium models can be efficient tools for CO_2 sequestration related optimization problems

Accomplishments to Date

- Completed review of existing CO_2 sequestration modeling approaches and their application to actual sites.
- Conducted modeling studies at 3 example sites.
- Developed and implemented:
  - Dynamic reconstruction for VI models
  - Vertical heterogeneity for VE models
  - algorithm for macroscopic invasion percolation modeling
  - new optimization algorithm for pressure management

Synergy Opportunities

- Criteria developed in this project may guide model approaches used in other projects
- New modeling and optimization capabilities are available

Future Plans

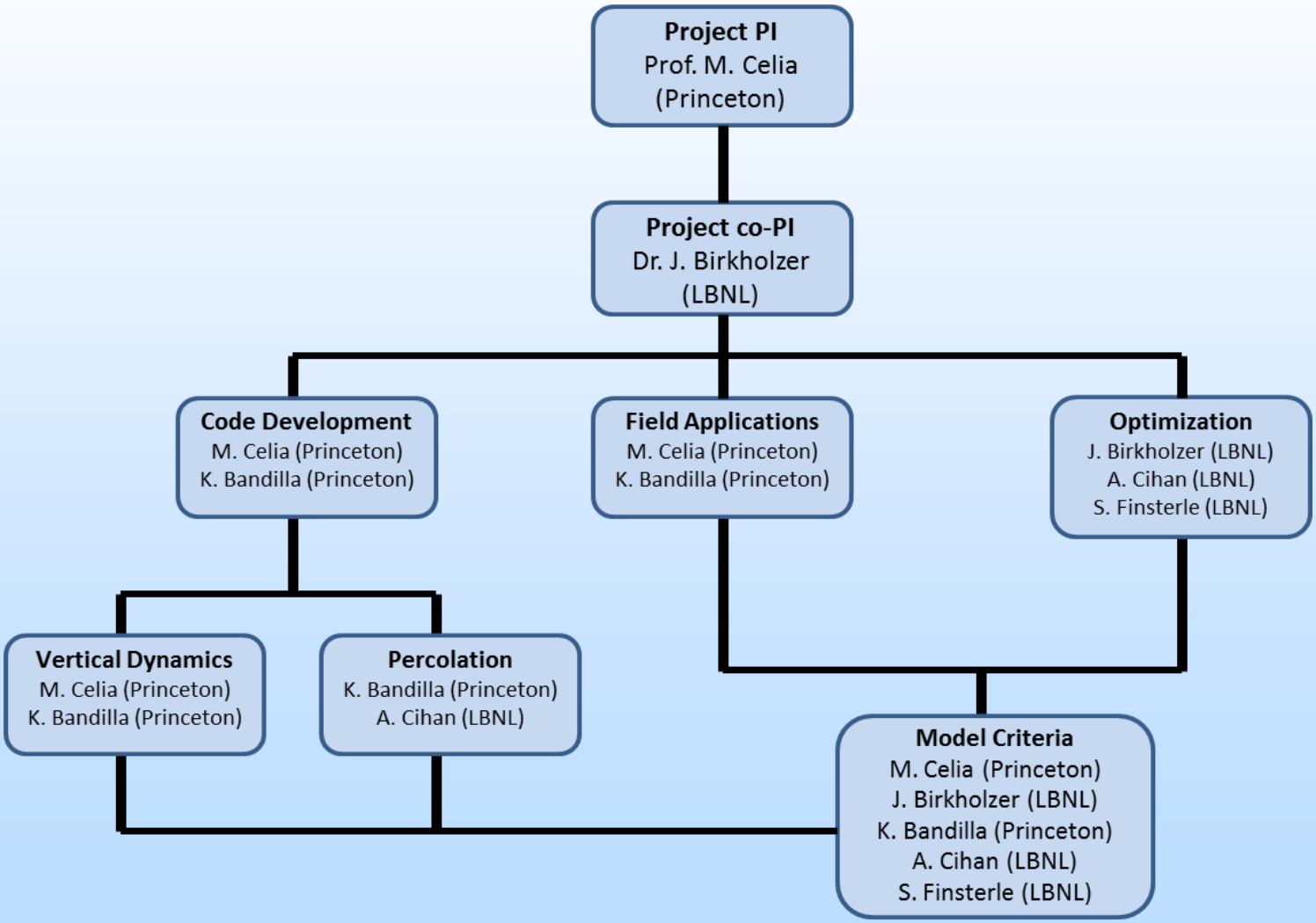
- Finish model comparison studies for Ketzin site
- Refinement of best practices guidelines for model complexity choice
- Prepare manuscript on vertically-integrated models with vertical heterogeneity
- Prepare final report

THANK YOU!

Karl Bandilla
Princeton University
bandilla@princeton.edu

Appendix

Organization Chart



Gantt Chart

	BP1 (2012-2013)				BP2 (2013-2014)				BP3 (2014-2015)				BP4 (2015-2016)			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1: Proj Mgmt and Planning																
Subtask 1.1: PMP And KickOff	MS															
Subtask 1.2: Project Planning and Reporting																
Task 2: Development Of New Models																
Subtask 2.1: Review And Analyze Existing Models			MS													
Subtask 2.2: Models with Vertical Drainage Dynamics				MS			MS									
Subtask 2.3: New Percolation Model					MS			MS								
Task 3: Model Existing Injection Operations					MS		MS	MS						MS		
Task 4: Optimization Models							MS		MS			MS				
Task 5: Criteria for Model Complexity														MS		MS

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

Bibliography 1

- Huang, X., Bandilla, K.W., Celia, M.A., Bachu, S., 2014. Basin-scale modeling of CO_2 storage using models of varying complexity. International Journal of Greenhouse Gas Control, 20, pp. 73-86.
- Guo, B., Bandilla, K.W., Doster, F., Keilegavlen, E., Celia, M.A., 2014. A Vertically-integrated Model with Vertical Dynamics for CO_2 storage. Water Resources Research, 50(8), pp. 6269–6284.
- Bandilla, K.W., Celia, M.A., Birkholzer, J.T., Cihan, A., Leister, E., 2014. Overview of approaches for modeling of geologic carbon sequestration in saline aquifers. Groundwater, .

Bibliography 2

- Bandilla, K.W., Celia, M.A., Leister, E., 2014. Impact of Model Complexity on CO_2 plume modeling at Sleipner. Energy Procedia, 63, pp. 3405-3415.
- Guo, B., Bandilla, K.W., Keilegavlen, E., Doster, F., Celia, M.A., 2014. Application of a vertically-integrated model with subscale vertical dynamics to field injection sites for CO_2 storage. Energy Procedia, 63, pp. 3523-3531.
- Cihan, A., Birkholzer, J.T., Bianchi, M., 2014. Targeted pressure management during CO_2 sequestration: Optimization of well placement and brine extraction in a heterogeneous aquifer. Energy Procedia, 63 pp. 5325-5332.

Bibliography 3

- Cihan, A., Birkholzer, J.T., Trevisan, L., Bianchi, M., Zhou, Q., Illangasekare, T., 2014. A connectivity-based upscaling-approach for modeling two-phase flow in heterogeneous geological formations. Energy Procedia, 63, pp. 3456-3463.
- Celia, M.A., Bachu, S., Nordbotten, J.M., Bandilla, K.W., 2015. Status of CO_2 Storage in Deep Saline Aquifers with Emphasis on Modeling Approaches and Practical Simulations. Water Resources Research, accepted.
- Cihan, A.J., Birkholzer, J.T., Bianchi, M., 2015. Optimal Well Placement and Brine Extraction for Pressure Management during CO_2 Sequestration. International Journal of Greenhouse Gas Control, accepted.

Bibliography 4

- Celia, M.A., Bandilla, K.W., 2015. Geological Sequestration of Carbon Dioxide. Handbook of Groundwater Engineering, accepted.
- Bo Guo, 2013. Inclusion of vertical dynamics in vertically integrated models for CO_2 storage. Presented at the 2nd International Conference on Non-Linearities and Upscaling in Porous Media in Bergen, Norway, September 30 – October 2.
- X. Huang, 2013. Basin-scale Modeling of Geological Carbon Sequestration: Model Complexity, Injection Scenario and Sensitivity Analysis. Presented at the American Geophysical Union Fall Meeting 2013 (December 9 – 13, San Francisco, CA).

Bibliography 5

- B. Guo, 2014. Multiscale Model with Vertical Dynamics in a Vertically-integrated Framework for CO_2 Storage. Presented at the International Conference on Computational Methods in Water Resources held in Stuttgart, Germany.
- K. Bandilla, 2014. A multi-tiered approach for carbon sequestration Area of Review delineation. Presented at the American Geophysical Union Science Policy 2014 conference in Washington, DC).

Bibliography 6

- Birkholzer, J.T., A. Cihan, M. Bianchi, 2014. Optimization of Well Placement and Brine Extraction for Pressure Control Along Critically Stressed Faults. Presented at the 13th Annual Conference on Carbon Capture, Utilization and Sequestration, Pittsburgh, PA, April 28-May 1.
- E. Leister, 2014. Evaluating Storage Model Complexity - CO_2 Plume Matching at Sleipner. Presented at the Environmental Engineering and Water Resources Brown Bag Seminar at Princeton University on April 18th.

Bibliography 7

- M. Celia, J. Nordbotten, K. Bandilla, S. Gasda, B. Guo, 2012. Multi-scale Modeling and Model Complexity in CO_2 Sequestration Simulations. Presented at American Geophysical Union 2012 Fall Meeting, San Francisco, CA, 3rd-7th of December.
- B. Guo, K. Bandilla, M. Celia, 2012. Inclusion of Vertical Dynamics in Vertically-integrated Models for CO_2 Storage. Presented at American Geophysical Union 2012 Fall Meeting, San Francisco, CA, 3rd-7th of December.

Bibliography 8

- M. Celia, 2013. Can CCS Find Synergies with Geothermal Energy and Shale Gas Production? Presented at SIAM Conference on Mathematical & Computational Issues in the Geosciences, Padua, Italy, June 17 – 20.
- K. Bandilla, 2013. Pressure uncertainty and the Implication for Risk. Presented at IEAGHG Combined Modelling and Risk Management Network Meeting, Trondheim, Norway, June 10 – 13.

Bibliography 9

- Bandilla, K.W.,2013. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long–term Fate. Presented at the DOE Carbon Storage R&D Review Meeting, Pittsburgh, PA, August 20 – 22.
- Birkholzer, J.T., 2013. Studies for Modeling CO_2 Processes: Pressure Management, Basin– Scale Models, Model Comparison, and Joint Inversion. Presented at the DOE Carbon Storage R&D Review Meeting, Pittsburgh, PA, August 20 – 22.

Bibliography 10

- Bandilla, K.W., 2013. Active pressure management through brine production for industrial-scale geologic carbon sequestration deployment in the Illinois Basin, USA. Presented at the DOE Carbon Storage R&D Review Meeting, Pittsburgh, PA, August 20 – 22.
- Guo, B., 2013. A vertically-integrated Model with Vertical Dynamics for CO_2 Storage. Presented at the Department of Mathematics at the University of Bergen, Bergen, Norway, September 25.

Bibliography 11

- Guo, B., 2013. Inclusion of vertical dynamics in vertically integrated models for CO_2 storage. Presented at the 2nd International Conference on Non-Linearities and Upscaling in Porous Media, Bergen, Norway, September 30 – October 2.
- Huang, X., 2013. Basin-scale Modeling of Geological Carbon Sequestration: Model Complexity, Injection Scenario and Sensitivity Analysis. Presented at the American Geophysical Union Fall Meeting 2013, San Francisco, CA, December 9 – 13.

Bibliography 12

- Guo, B., 2014. Multiscale Model with Vertical Dynamics in a Vertically-integrated Framework for CO_2 Storage. Presented at the International Conference on Computational Methods in Water Resources, Stuttgart, Germany.
- Bandilla, K., 2014. A multi-tiered approach for carbon sequestration Area of Review delineation. Presented at American Geophysical Union Science Policy 2014, Washington, DC.

Bibliography 13

- Bandilla, K.W., 2014. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate. Presented at the DOE Carbon Storage R&D Project Review Meeting, Pittsburgh, PA, August 12 - 14.
- Birkholzer, J.T., 2014. Studies for Modeling CO_2 Processes, Comparison, and Joint Inversion with Characterization and Monitoring Data. Presented at the DOE Carbon Storage R&D Project Review Meeting, Pittsburgh, PA, August 12 - 14.

Bibliography 14

- Bandilla, K.W., 2014. Modeling CO_2 migration at Sleipner using models of varying complexity. Presented at the American Geophysical Union Fall Meeting 2014, San Francisco, CA, December 15 – 19.
- Cihan, A., 2014. A Constrained Differential Evolution algorithm for reservoir management: optimal placement and control of wells for geological carbon storage with uncertainty in reservoir properties. Presented at the American Geophysical Union Fall Meeting 2014, San Francisco, CA, December 15 – 19.

Bibliography 15

- Guo, B., 2014. A multi-layer vertically integrated model with vertical dynamics and heterogeneity for CO_2 sequestration . Presented at the American Geophysical Union Fall Meeting 2014, San Francisco, CA, December 15 – 19.
- Celia, M.A., 2015. Model Complexity and Simulation Approaches for Geological Sequestration of Carbon Dioxide. Presented at both the City University of Hong Kong (1/23) and at the Polytechnic University of Hong Kong (1/26).

Bibliography 16

- Celia, M.A., 2015. Leakage along Old Wells with Applications to CO_2 Sequestration and Methane Emissions. Presented at the University of Kansas, February 19.
- M.A. Celia, 2015. Leakage along Old Wells with Applications to CO_2 Sequestration and Methane Emissions. Presented at the Division of Earth Sciences, Lawrence Berkeley National Laboratory.
- M.A. Celia, 2015. Carbon Capture and Storage. Presented at the University of Bergen Summer School on Sustainability, Bergen, Norway.

Bibliography 17

- Celia, M.A., S. Bachu, J.M. Nordbotten, and K.W. Bandilla, 2015. Status of CO_2 Storage in Deep Saline Aquifers with Emphasis on Modeling Approaches and Practical Simulations. *Water Resources Research*, 51(9), p. 6846–6892.
- Cihan, A.J., J.T. Birkholzer, and M. Bianchi, 2015. Optimal Well Placement and Brine Extraction for Pressure Management during CO_2 Sequestration. *International Journal of Greenhouse Gas Control*, 42, p. 175–187.

Bibliography 18

- Cihan, A., J.T. Birkholzer, and M. Bianchi, 2015. Pressure Management during Geological CO_2 Sequestration: Optimal Well Placement and Brine Extraction. *Proceedings of the TOUGH Symposium*, Lawrence Berkeley National Laboratory, Berkeley, CA.
- Oldenburg, C., S. Mukhopadhyay, and A. Cihan, 2015. On The Use of Darcy's Law and Invasion-Percolation Approaches for Modeling Large-Scale Geologic Carbon Sequestration. *Greenhouse Gases: Science and Technology*, 6 (1), p. 19–33.

Bibliography 19

- Celia, M.A., and K.W. Bandilla, 2015. Geological Sequestration of Carbon Dioxide. *Handbook of Groundwater Engineering*, accepted.
- B. Guo, 2015. Axisymmetric flows from fluid injection into a confined porous medium. Presented at the Non-linearities and Upscaling in Porous Media Conference in Freudenstadt, Germany (9/8 – 9/12/2015).
- M. A. Celia, 2015. CCS: Current Status, Future Prospects, and the Role of NUPUS. Presented at the Non-linearities and Upscaling in Porous Media Conference in Freudenstadt, Germany (9/8 – 9/12/2015).

Bibliography 20

- B. Guo, 2015. Flow regimes for fluid injection into a confined aquifer - implications to geological CO_2 sequestration. Presented at the School of Environmental Science and Engineering, China Ocean University, Shandong.
- B. Guo, 2015. Multiscale vertically-integrated models for CO_2 sequestration in saline aquifers. Presented at the Institute of Mechanics, Chinese Academy of Sciences, Beijing.

Bibliography 21

- B. Guo, 2015. Multiscale modeling Approaches for CO_2 injection and migration. Presented at the International Congress on Industrial and Applied Mathematics in Beijing, China and at the Department of Hydraulic Engineering, Tsinghua University, Beijing, China.
- M. A. Celia, 2015. Modeling Approaches for CO_2 Injection in Conventional and Unconventional Reservoirs. Presented at the PetroChina Research group in Beijing, China.

Bibliography 22

- M. A. Celia, 2015. Carbon Dioxide Sequestration in Conventional and Unconventional Reservoirs. Presented at the Department of Hydraulic Engineering, Tsinghua University, Beijing, China.
- K. W. Bandilla, 2015. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate. Presented at the Carbon Storage R&D Project Review Meeting in Pittsburgh, Pa.

Bibliography 23

- K. Bandilla, 2015. Impact of model complexity for carbon dioxide migration in structured heterogeneous domains. Presented at the 2015 American Institute of Chemical Engineering Annual Meeting in Salt Lake City, UT (11/8-11/13/2015).
- K. Bandilla, 2015. Vertically-integrated Approaches for Carbon Sequestration Modeling. Presented at the 2015 American Geophysical Union Fall Meeting in San Francisco, CA (12/14-12/18/2015).
- B. Guo, 2015. Flow regime analysis for fluid injection into a confined aquifer: implications for CO_2 sequestration. Presented at the 2015 American Geophysical Union Fall Meeting in San Francisco, CA (12/14-12/18/2015).

Bibliography 24

- A. Cihan, 2015. Determining the Area of Review (AoR) in Carbon Capture and Storage: A tiered, probabilistic methodology to generate risk map. Presented at the 2015 American Geophysical Union Fall Meeting in San Francisco, CA (12/14-12/18/2015).
- B. Becker, 2015. Evaluation of the Coupling of a Full-Dimensional Multiphase Model with a Vertical Equilibrium Model for the Simulation of Underground Gas Storage. Presented at the 2015 American Geophysical Union Fall Meeting in San Francisco, CA (12/14-12/18/2015).

Bibliography 25

- Cihan, A., and J. T. Birkholzer, 2015. Optimization of Fluid Injection and Extraction in Deep Subsurface Reservoirs: Examples from CO_2 Sequestration. Presented at the Technical Workshop on Enhanced Water Recovery, Livermore, CA (9/14/2015).
- Guo, B., K. W. Bandilla, J. M. Nordbotten, M. A. Celia, E. Keilegavlen, F. Doster, 2016. Multiscale multilayer vertically-integrated model with subscale vertical dynamics for CO_2 migration in heterogeneous formations. Revision submitted to *Water Resources Research*.

Bibliography 26

- Guo, B., Z. Zheng, K. W. Bandilla, M. A. Celia, H. A, Stone, 2016. Flow regime analysis for geologic CO_2 sequestration and other subsurface fluid injections. Revision submitted to the *International Journal of Greenhouse Gas Control*.
- K. Bandilla, 2016. Applicability of vertically integrated models for carbon storage modeling in structured heterogeneous domains. Presented at the XXI International Conference of Computational Methods in Toronto, Canada (6/20-6/24/2016).

Bibliography 27

- B. Guo, 2016. Multiscale Vertically-integrated Models with Vertical Dynamics for CO_2 migration in Heterogeneous Geologic Formations. Presented at the XXI International Conference of Computational Methods in Toronto, Canada (6/20-6/24/2016).
- B. Guo, 2016. Flow regime analysis for geologic CO_2 sequestration and other subsurface fluid injections. Presented at the XXI International Conference of Computational Methods in Toronto, Canada (6/20-6/24/2016).