KIGAM Korea Institute of Geoscience and Mineral Resources

INTERNATIONAL SCHOOL FOR GEOSCIENCE RESOURCES (IS-Geo)
KOREA INSTITUTE OF GEOSCIENCE AND MINERAL RESOURCES (KIGAM)

INTENSIVE TRAINING COURSE ON
CO_2 School – Carbon Capture, Utilization and Storage

The **International School for Geoscience Resources** of KIGAM presents an intensive training course on **"CO_2 School – Carbon Capture, Utilization and Storage"**. The course will take place at the Ara room of International School for Geoscience Resources of KIGAM in Daejeon (Korea) in **November 4 - 15, 2013** and will include the following modules:

Module	Date	Instructors
Module 1. Overview of CCUS and various aspects of numerical modeling Topic 1. Overview of CCUS and introduction to numerical modeling Topic 2. Physical and chemical processes of geological carbon sequestration Topic 3. Numerical methods Topic 4. Model parameterization and uncertainty quantification Topic 5. Scale issues in geological carbon sequestration modeling	Nov. 4 - 8	Timothy Scheibe (PNNL)
Module 2. Pilot sites and related subsurface applications Topic 1. Overview of the geologic storage of CO_2 in sedimentary reservoirs Topic 2. Geologic storage of CO_2 in non-sedimentary reservoirs and in Enhanced Oil Recovery Projects (CO_2 EOR) Topic 3. Monitoring CO_2 storage sites and CO_2 EOR sites Topic 4. Public engagement and success of pilot sites Topic 5. Shale-Gas reservoirs: exploration, hydraulic fracturing, and potential for CO_2 storage and secondary recovery	Nov. 4 - 8	Charlotte Sullivan (PNNL)

Module 3. Subsurface Transport Over Multiple Phases (STOMP) Simulator Topic 1. Introduction to multifluid subsurface modeling with STOMP Topic 2. Benchmark problems for geologic sequestration in deep saline formations Topic 3. Reservoir-Scale problems for geologic sequestration in deep saline reservoirs with coupled well models Topic 4. Geochemical modeling of saturated and CO_2 sequestration systems Topic 5. Viscous fingering of dissolved CO_2 and geomechanical modeling of geologic sequestration systems	Nov. 11-15	Mark White/ Signe White (PNNL)

COURSE INFORMATION

- ### Agenda
  - This course will provide the participants with a general introduction to Carbon Capture Utilization and Storage (CCUS). And it gives eologic and other background material and examples for many of the technical topics covered in CCUS. This course will also provide a general introduction to STOMP, a multifluid subsurface flow and reactive transport simulator, developed at the Pacific Northwest National Laboratory (PNNL), with specific attention to the STOMP-CO2 and -CO2e operational modes of the simulator. It is for computer laboratories with a series of topics concerned with the modeling of CO_2 sequestration in geologic reservoirs.

- ### Course Covered
  - Module 1 will provide the participants with a general introduction to Carbon Capture Utilization and Storage (CCUS). So it will contain motivation for CCUS, discussion of critical social and technical issues, and an overview of proposed solution approaches. And it will do them the background understanding necessary to effectively apply numerical models to carbon sequestration problems, and will prepare students for the STOMP modeling short course to be offered the following week.
  - Module 2 will provide them with a background understanding of the geologic, characterization, and social issues involved in siting and operating CCS and CCUS projects, and an understanding of the sources of data for building geologic and numerical models. So this module occurs module 2 for

synergy effects by giving geologic and other background material and examples for many of the technical topics covered in Module 2 to the participants.
- Module 3 will provide them with a general introduction to STOMP, a multifluid subsurface flow and reactive transport simulator, developed at the Pacific Northwest National Laboratory (PNNL), with specific attention to the STOMP-CO2 and -CO2e operational modes of the simulator.

Course Requirements: Prerequisite

- The participants should have a background in one of the following fields: Geology, Geochemistry, Geophysics, Geomechanics, basics of Petroleum Geology or other Earth Science disciplines and numerical methods for partial differential equations.
- The participants must have a good knowledge of the English language as the course will be conducted in English as well as using the computer.

Who should Attend?

- This course is designed for scientists, researchers, engineers involved in CO_2 studies with special emphasis on those interested in engineering or geological applications of CO_2, or both in the academic, public and the private consultant sectors.

Module 1. Overview of CCUS and Various Aspects of Numerical Modeling – Dr. Timothy Scheibe

- ## Summary of Module Contents and Learning Objectives

This module will provide the participants with a general introduction to Carbon Capture Utilization and Storage (CCUS). The introductory material will include motivation for CCUS, discussion of critical social and technical issues, and an overview of proposed solution approaches. Following this introduction, the remainder of the module will focus on numerical modeling approaches and methodologies that are being used to evaluate, design and monitor implementations of geologic storage of CO_2 (carbon sequestration). This module will be coordinated with Module 2 to provide the participants a practical application-based context for the numerical modeling methods being presented. In addition to presenting the current state-of-the-art of simulation technologies, this module will also introduce participants to a number of important science questions that are guiding current research and model development in geological carbon sequestration.

- ## Day 1. Overview of CCUS and Introduction to Numerical Modeling

The opening day will provide the students with a general introduction to the problem of increasing atmospheric carbon dioxide (CO_2), and to Carbon Capture, Utilization and Storage (CCUS) as one part of a strategy to mitigate CO_2 accumulation. The general introduction will focus on the scope of the global CCUS problem and motivate the need for reliable numerical simulation tools to assess and design site-specific implementations of geological carbon sequestration.

- Introduction to CCUS and the Global Carbon Challenge
- Field-Scale Simulation Tools for Geological Carbon Sequestration
- Data Management, Workflow Management, and Visualization

- ## Day 2. Physical and Chemical Processes of Geological Carbon Sequestration

The second day of the module will focus on conceptual and mathematical descriptions of those physical and chemical processes that play significant roles in geological carbon sequestration. Key processes and conceptualizations to be presented include multiphase flow in porous media, phase transitions and inter-phase dissolution, equations of state, density-driven flow, brine acidification and chemical reactions, and geomechanical deformations coupled to flow. These will be presented in terms of general conceptualizations of the processes as well as specific mathematical representations commonly used in formulating numerical simulators. The three lectures will be organized by general classes of processes (lecture 1: physical flow processes; lecture 2: biogeochemical reaction processes; lecture 3: geomechanical processes).

- Multiphase Flow in Natural Porous Media
- Brine Acidification and Biogeochemical Reactions
- Geomechanical Deformation Coupled to Multiphase Flow

• Day 3. Numerical Methods

The third day of the module will focus on numerical methods that are used to solve the partial differential equations (PDEs) and other equations that arise from the conceptual models and theories presented on Day 2. The first lecture will address methods of discretising PDEs, which convert them into systems of linear and non-linear algebraic equations. The lecture 2 addresses methods of obtaining solutions to these (typically large) systems of equations. In cases where these systems of equations become extremely large (with hundreds of thousands to hundreds of millions of unknowns), high-performance computing methods can be applied to facilitate timely solution. Parallelization and high-performance computing will be addressed in the third lecture.

- Spatial and Temporal Discretization Methods
- Solution of Large Systems of Linear and Non-Linear Equations
- High-Performance Computing Applications

• Day 4. Model Parameterization and Uncertainty Quantification

The fourth day of the module will focus on a wide range of issues associated with reservoir characterization and selection of model parameters. The lecture 1 will provide an overview of a variety of approaches commonly used in model parameterization and an introduction to associated issues and problems. The lecture 2 will introduce specific methodologies of calibration, inverse modeling and data assimilation, and the third lecture will address sources of model predictive uncertainty (both parametric uncertainty and structural uncertainty) and new developments in quantifying and reducing uncertainty.

- Approaches to Model Parameterization
- Model Calibration and Inverse Modeling
- Uncertainty Quantification

• Day 5. Scale Issues in Geological Carbon Sequestration Modeling

The fifth day of the module will shift to a more fundamental perspective of processes involved in carbon sequestration. In particular, we will examine processes at a range of scales that are smaller than those resolved by commonly-used simulators, specifically from the molecular scale to the pore scale. This set of lectures will provide the participants with deeper understanding of fundamental processes and how they relate to model conceptualizations at larger scales. The lecture 1 will focus on fundamental process descriptions and their impact on larger-scale phenomena, and will also present some experimental methods used to elucidate these processes. The lecture 2 will introduce a class of simulation tools designed to simulate multiphase flow, transport, and reaction processes at a detailed level. The final lecture will discuss linkages between these detailed process models and more conventional reservoir-scale simulators, including some new directions in multiscale simulation.

- Molecular and Pore-Scale Processes in CO2 Sequestration
- Pore-Scale Simulation Methods
- Linking Sub-Grid Processes to Reservoir-Scale Simulators

Module 2. Pilot Sites and Related Subsurface Applications – Dr. Charlotte Sullivan

• Summary of Module Contents and Learning Objectives

This module provides the participants with geologic and other background material and examples for many of the technical topics covered in Module 2. The introductory lecture will include a review of the important factors in site selection for geologic storage of carbon dioxide; a brief review of social issues; and a risk-based approach to selection, characterization, monitoring, and closure of CCS sites. Following this introduction, the remainder of the lectures will provide the participants with a practical, application-based context for the numerical modelling methods being presented in Module 2-1. Lecture topics for this module include differences in storage of CO_2 in carbonate, sandstone, and reactive reservoirs such as basalts. Separate lectures will cover Carbon Capture and Utilization (CCUS), primarily in CO_2 enhanced oil recovery (CO_2 EOR), with emphasis on application in the SE Asian and Pacific realms; and monitoring technologies to detect and mitigate potential for induced seismicity and leakage from the storage reservoir. The importance of public engagement will be explored with examples, and finally we will cover aspects of shale-gas exploration and production; hydraulic fracturing; and secondary recovery and CO_2 storage potential in shales and coal-bed methane reservoirs.

• Day 1. Overview of the Geologic Storage of CO_2 in Sedimentary Reservoirs

The opening day will provide the participants with a general introduction to regional natural and anthropogenic CO_2 sources and potential geologic sinks; site screening and site selection for geologic storage of CO_2 (Carbon Capture and Storage - CCS); the differences between CCS and CCUS (Carbon Capture and Utilization); and the peculiarities and challenges of carbon dioxide storage in the most common sedimentary rock reservoirs. The introductory lecture will focus on site selection and concepts of reducing geologic uncertainty and risk in CCS. The Lecture 2 will provide an overview of CO_2 storage in carbonate reservoirs, and following lecture will examine geologic storage in carbonate reservoirs and sandstone reservoirs with relevant examples.

- Site Screening, Site Selection and Risk Reduction
- CO_2 Storage in Carbonate Reservoirs - with aspects relevant to SE Asian and Pacific Realms
- CO_2 Storage in Sandstone Reservoirs - with aspects relevant to SE Asian and Pacific Realms

- **Day 2. Geologic Storage of CO_2 in Non-Sedimentary Reservoirs and in Enhanced Oil Recovery Projects (CO_2 EOR)**

The second day will provide the participants with an overview of CO_2 storage in "unconventional" non-sedimentary reservoirs, as well as the basics, efficiency, and challenges of CO_2 storage in enhanced oil recovery (EOR) reservoirs. The lecture 1 will explore the special case of mineral trapping of CO_2 in basalts, and the potential for offshore storage. Lecture 2 will examine the differences between CO_2 storage in saline reservoirs and CO_2 utilization in enhanced oil recovery, and Lecture 3 will examine the potential and challenges of CO_2 storage and enhanced oil recovery in our regional areas of interest.

  - CO_2 Storage in Basalts and Fractured Crystalline Rock, Onshore and Offshore
  - CCUS and CO_2 Enhanced Oil Recovery (CO_2 EOR)
  - Challenges of CO_2 Storage and CO_2 EOR in SE Asian and Pacific Realms

- **Day 3. Monitoring CO_2 Storage Sites and CO_2 EOR Sites**

The third day will explore the motivation and methods for monitoring active and post-closure sites, as well as the types of data generated by different monitoring technologies. We will also discuss mitigation technologies and strategies. The lecture 1 will introduce the objectives and tools of monitoring, standard borehole technologies, and the differences for CCS and CCUS sites. The lecture 2 will cover microseismic monitoring, and time-lapse 2D, 3D, vertical seismic profiling (VSP), and cross-well seismic technologies. The third lecture will examine electrical-resistivity-based (ERT) monitoring and site-wide surface deformation monitoring.

  - Introduction to Monitoring CCS and CCUS sites
  - Geophysical Monitoring
  - Other Monitoring Technologies

- **Day 4. Public Engagement and Success of Pilot Sites**

The fourth day will provide the participants with the insights into the critical role of public engagement, with examples of successful projects and projects that were adversely impacted or were terminated due to negative public perception. The lecture 1 will introduce the elements and best practices of successful public engagement. The lecture 2 will present public engagement case histories and include discussion of possible cultural differences in public perception. The Lecture 3 will review and summarize important elements of site selection, characterization, operation, and closeout of CCS and CCUS projects, and will include time for discussion of special topics of interest.

  - Public Engagement Introduction and Best Practices
  - Public Engagement Case Histories

- Summary of CCS/CCUS Site Selection, Characterization, Monitoring, and Site Closure

- **Day 5. Shale-Gas Reservoirs: Exploration, Hydraulic Fracturing, and Potential for CO_2 Storage and Secondary Recovery**

The final day for this module will provide the participants with an overview of shale-gas reservoirs; including the history of their development, myths and realities of hydraulic "fracking", and the potential for CO_2 enhanced secondary recovery, and for CO_2 storage in depleted shale-gas or coal-bed methane wells. The lecture 1 will explore the origin and distribution of shale-gas reservoirs, and the potential for shale-gas reservoir development in our regions of interest. The lecture 2 will review hydraulic fracturing technology and associated environmental impacts. The lecture 3 will examine recent research into the feasibility of using anthropogenic CO_2 to enhance natural gas recovery and the feasibility of storing large volumes of CO_2 in pressure-depleted shale-gas wells as well as in coal-bed methane reservoirs.

- Introduction to Shale-Gas, Origin and History of Development.
- Shale-Gas Reservoirs and Hydraulic Fracturing
- Shale-Gas and Coal-Bed Methane- Secondary Recovery and CO_2 Storage

Module 3. Subsurface Transport Over Multiple Phases (STOMP) Simulator – Dr. Mark White and Ms. Signe White

- ### Summary of module content and learning objectives

This module will provide the participants with a general introduction to STOMP, a multifluid subsurface flow and reactive transport simulator, developed at the Pacific Northwest National Laboratory (PNNL), with specific attention to the STOMP-CO2 and -CO2e operational modes of the simulator. The participants will be guided by two instructors from the STOMP development team, using lectures and computer laboratories, through a series of topics concerned with the modeling of CO_2 sequestration in geologic reservoirs. This module requires the participants to work through a series of problems and exercises, designed to demonstrate the simulator's features and capabilities. The participants will learn to prepare input files for geologic sequestration problems and interpret simulation results by working with sample problems that vary in complexity and structure. The sample problems are designed to emphasis specific features of the simulator, demonstrate the modeling of geologic sequestration processes, and serve as prototypes and templates for applications for the students after the course. Lectures will be used to describe the mathematical models, numerical solution approaches, and code structure, but will also cover a series of simulation applications conducted by the PNNL. This module will be taught in a computer laboratory with the participants working in pairs to compile and execute numerical simulations, subsequently convert simulation results to visual form and analyse the generated results. This module will then be challenged with problem variants to expand their numerical simulation capabilities and understanding.

- ### STOMP Overview

The STOMP simulator is a suite of computer codes, designated as operational modes, for solving subsurface multifluid flow and reactive transport problems. Operational modes are distinguished by the solved conservation equations and vary in complexity from those involving the isothermal flow of water and dilute solutes with a passive gas, to those involving flow and heat transport for three mobile and three immobile phases. The STOMP simulator has been applied to support laboratory and field investigations of: geologic nuclear waste repositories; radionuclide transport; unsaturated zone hydrology; reactive barriers; nuclear waste tank thermal histories; surface barriers; freeze walls; soil desiccation; soil vapor extraction; volatile organic migration and fate; dense nonaqueous phase migration and natural attenuation; geologic sequestration of greenhouse gases; coupled reactive transport; oil shale production; and natural gas hydrate production. STOMP's capabilities and numerical schemes continue to be developed with the current emphasis being gas hydrate production via CO_2 injection, oil shale production, and coupled geomechanical modeling. During the short course students will work with the sequential implementation of the simulator. A suite of demonstration problems have been developed for the short course, which include problems involving multifluid flow, heat transport, nonaqueous phase liquids, salt-water intrusion, geologic sequestration, gas hydrate production, and geochemistry. A subset of these problems will be covered during the course, but students will be encouraged to explore the remaining problems or develop their own problems at the end of the course.

- **Day 1. Introduction to Multifluid Subsurface Modeling with STOMP**

The opening day of the STOMP module will be used to orient the participants to the simulator, with a focus on understanding its capabilities, specifying input, prescribing output, executing the code, interpreting results and errors, and converting and plotting output. This module will open with an overview lecture, followed by the students working with the simulator on three problems involving isothermal flow and nonreactive transport in variably saturated geologic media. All problems conducted in the first day will use the STOMP-W operational mode. The number of problems addressed will depend on the participants' pace. The day will close with participants' workshop where participants will be free to work on unfinished problems or explore new problems of their own. The module instructors will be available during the workshop for mentoring.

- STOMP Overview Lecture
- Building Input Files
- Understanding Output Files
- Converting Output Files for Result Visualization
- Solute Transport and Two-Phase Heat Transfer Problems
- Participants' Workshop
- Aqueous Flow in Saturated and Unsaturated Porous Media : The user is introduced to the development of input files for successful simulation of flow problems. The first problem is a simple 1D vertical, single-phase aqueous flow system. Through manipulation of input file parameter values and boundary conditions, various saturated and unsaturated systems are obtained.
- Aqueous Flow to a Well in a Confined Multi-Layer System : This test case illustrates flow to a well in a confined multi-layer system, where two identical aquifers (upper and lower) are separated by an aquitard. The well produces only from the lower aquifer, where it is fully penetrating. This problem is known in the literature as the leaky aquifer problem. The user is introduced to a two-dimensional domain, a cylindrical coordinate system, and Neumann boundary conditions.
- Simulation of Counter-Current Flow and Heat Transport with Local Evaporation and Condensation (Natural Heat Pipe) : This heat pipe problem demonstrates the simulator's ability to model counter-current aqueous and

gas flow in variably saturated geologic media, including saturations below residual saturation. As posed, the problem involves one-dimensional horizontal flow and heat transport, but this classic multifluid subsurface flow and transport problem involves complex flow behavior, which is subtle to changes in soil properties. The user will first explore the affects of changes in soil thermal conductivity, specific heat, and enhanced vapor transport on the formation and temperature distribution for a horizontal one-dimensional heat pipe. After completing these investigations the user is asked to design an input file for a two-dimensional problem involving dynamic heat pipe flow.

- **Day 2. Benchmark Problems for Geologic Sequestration in Deep Saline Formations**

The second day will continue to reinforce the topics covered in the first day, but with the simulation focus being on carbon sequestration. The day will open with an overview lecture on carbon sequestration modeling activities at PNNL. Following the opening lecture, a review session will be held on prescribing initial conditions, boundary conditions, and sources, with an emphasis on understanding STOMP's capabilities. As part of this review session, the coupled-well model and vertical equilibrium models will be described. The remainder of the day will be spent with the students working through problems involving the sequestration of carbon dioxide in deep saline reservoirs. The solved problems are benchmark problems selected from model comparison studies published in the literature or problems designed to highlight the unique features of the coupled well model or vertical equilibrium model. The focus on this day will be isothermal and nonisothermal multiphase flow for geologic sequestration. The number of problems addressed will depend on the participants' pace. The day will close with participants' workshop where participants will be free to work on unfinished problems or explore new problems of their own. The module instructors will be available during the workshop for mentoring.

- STOMP-CO2 and -CO2e Overview Lecture
- Equation of State
- Initial and Boundary Conditions
- Sources and the Coupled-Well Model
- Benchmark Geologic Sequestration Problems
- Participants' Workshop
- Discharge of Sequestered CO_2 along a Fault Zone (GeoSeq #4) : Loss of CO_2 from a deep fresh-water aquifer through a leaky fault is investigated. This problem is identical to Problem 4 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002) and addresses two-fluid flow of CO_2 and aqueous for a simplified one-dimensional vertical flow geometry. The problem is designed to investigate the transport of CO_2 from the disposal aquifer to another aquifer 500 m above, through an intersecting

vertical fault. The vertical fault is idealized using a one-dimensional geometry and constant pressure boundary conditions (Pruess and Garcia, 2002).

※ Pruess K., J. García, T. Kovscek, C. Oldenburg, J. Rutqvist, C. Steefel, and T. Xu. 2002. *Intercomparison of Numerical Simulation Codes for Geologic Disposal of* CO_2. LBNL-51813, Lawrence Berkeley National Laboratory, Berkeley, California.

- CO_2 Injection into a 2-Dimensional Layered Brine Formation (GeoSeq #7) : Pressure and buoyancy driven migration of CO_2 injected into a layered formation that is representative of the Sleipner Vest field in the Norwegian sector of the North Sea is investigated. This problem is identical to Problem 7 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002). A key assumption for the problem, as posed, was isothermal conditions at the formation temperature of 37˚C; therefore, STOMP-CO2 is executed for these simulations. The problem involves a constant mass rate injection of $scCO_2$ into a layered saline formation comprising sands and shales. There are five sand layers and four thinner shale layers, whose intrinsic permeability is lower than those of the sands. Students will be challenged in this problem to investigate grid convergence. The objective here will be for the students to develop a computational grid for the problem that minimizes execution time without altering the solution.

※ Pruess K., J. García, T. Kovscek, C. Oldenburg, J. Rutqvist, C. Steefel, and T. Xu. 2002. *Intercomparison of Numerical Simulation Codes for Geologic Disposal of* CO_2. LBNL-51813, Lawrence Berkeley National Laboratory, Berkeley, California.

- Contrasting Pressure- and Flow-Controlled CO_2 Injection Wells : The rate of CO_2 injection into saline reservoirs is often limited by the local fracture pressure gradient in the effort to meet regulatory requirements and to avoid fracturing the reservoir or caprock. This problem demonstrates the use of the coupled well model in STOMP-CO2, in which the user can specify both an injection rate and a maximum injection pressure. CO_2 is injected into a layered saline reservoir with layers of varying permeability and scenarios of pressure-controlled and flow-controlled CO_2 injection are investigated.
- Calculation of the Area of Review (AoR) : Delineating the Area of Review (AoR) of the injected CO_2 plume is required in the U.S. Environmental Protection Agency permit application for underground injection control (UIC) Class VI wells. A common approach for determining the extent of the separate phase CO_2 plume is to use the maximum extent based on gas saturation. However, factors that make saturation-based approach unreliable are 1) the gas saturation is dependent on rock porosity; 2) the gas density is dependent on pressure and temperature; and 3) any CO_2 saturation value defined as the cut-off point would be arbitrary. Consequently, the CO_2 plume extent based on CO_2 saturation may be misleading especially for rocks with very low

porosity. In addition, because of the potential for fingering and narrow channeling of CO_2 in continuous layers of relatively high permeability, the CO_2 plume extent determined using this approach may be controlled by preferential flow through fingers or channels.

- **Day 3. Reservoir-Scale Problems for Geologic Sequestration in Deep Saline Reservoirs with Coupled Well Models**

The third day will emphasize simulating reservoir-scale problems for geologic sequestration in deep saline reservoirs. During this day the students will be required to put into practice the techniques that they learned during the first two days, but on problems that are more complex, larger in scale, and more representative of reservoir systems than the benchmark problems. To keep the simulation times reasonable for the venue, the problems will be executed on coarse grids or two-dimensional realizations. The first problem will investigate the application of the coupled-well model to two reservoir conditions, yielding flow-controlled and pressure-controlled wells. The students will be challenged to find solutions to an injection problem where the reservoir is pressure-controlled, therefore restricting the CO_2 injection rate. The second problem will consider the leakage of CO_2 from a lower reservoir to an upper reservoir. The final problem is an assessment of storage capacity for a faulted reservoir with heterogeneous properties. This system will be modeled using a three-dimensional grid and the vertical-equilibrium transformation to a two-dimensional domain. Problems will require the application of both STOMP-CO2 and STOMP-CO2e. The number of problems addressed will depend on the students' pace. The day will close with a student workshop where students will be free to work on unfinished problems or explore new problems of their own. The course instructors will be available during the workshop for mentoring.

- Geologic Sequestration Applications Lecture
- Velo Collaborative Framework Overview and Demonstration
- Reservoir-Scale Geologic Sequestration Problems
- Participants' Workshop
- CO_2 Injection into a Hybrid Heterogeneous Domain : Geophysical field measurements combined with geostatistical techniques can yield complex geological models that have fully heterogeneous distributions of petrophysical properties. Typically only a limited number of parameters are distributed across the domain in a fully heterogeneous manner, such as porosity and intrinsic permeability. Parameters that define the relationships between capillary pressure, phase saturation, and phase relative permeability (ksP functions), are generally determined from measurements on discrete core samples. The STOMP simulator input routines have been designed to handle homogeneous, zoned, heterogeneous, and hybrid heterogeneous distributions of petrophysical properties. This problem

considers the injection of CO_2 into a saline formation whose petrophysical properties of porosity and intrinsic permeability are fully heterogeneous, ksP function parameters are zoned, and all other parameters homogeneous, the hybrid heterogeneous distribution.

- CO_2 Plume Evolution and Leakage through an Abandoned Well (Stuttgart #1a) : This problem involves the injection of scCO_2 into a saline formation with an abandoned well that provides a conduit for CO_2 migration between lower and upper permeable layers. Two scenarios are considered: 1a) deep conditions where the entire domain remains under supercritical temperature and pressure conditions for CO_2, and 1b) shallow conditions where the upper portion of the domain is outside of supercritical temperature and pressure conditions for CO_2. This problem is identical to Problem 1a from the series of problems developed at the University of Stuttgart (Ebigbo et al., 2007a,b), entitled "Numerical Investigations of CO_2 Sequestration in Geological Formations: Problem-Oriented Benchmarks. This problem was developed using analytical and semi-analytical solutions published by Nordbotten et al. (2004, 2005a,b). The deep scenario involves isothermal conditions and was executed with STOMP-CO2. This problem can be developed in two- and three-dimensional form. Students will first work with a two-dimensional version of the problem and then convert the problem to three-dimensional form for execution overnight. One objective of the problem will be for the students to evaluate the differences in the plume migration between the two- and three-dimensional domains.
- Estimating the CO_2 Storage Capacity of a Geological Formation (Stuttgart #3) : This problem investigates the storage capacity of a formation off the coast of Norway. The computational domain, intrinsic permeability distribution, and porosity distribution were provided as a benchmark problem; Problem 3 from the series of problems developed at the University of Stuttgart (Class et al., 2009), entitled "Numerical Investigations of CO_2 Sequestration in Geological Formations: Problem-Oriented Benchmarks. Four scenarios are considered: 1) injection into a single layer of the formation without hysteresis with a source injection, 2) injection into a single layer of the formation without hysteresis with a coupled-well model, 3) injection into a single layer of the formation with hysteresis, and 4) injection into the full domain without hysteresis, using a vertical equilibrium assumption. The students will be required to work with external data files for the computational domain and property distributions.

※ Class, H. A. Ebigbo, R. Helmig, H. K. Dahle, J. M. Nordbotten, M. A. Celia, P. Audigane, M. Darcis, J. Ennis-King, Y. Fan, B. Flemisch, S. E. Gasda, M. Jin, S. Krug, D. Labregere, A. N. Beni, R. J. Pawar, A. Sbai, S. G. Thomas, L. Trenty, L. Wei. 2009. "A benchmark

study on problems related to CO_2 storage in geologic formations. Summary and discussion of results." *Comput. Geosci.*, 13:409-434.

Day 4. Geochemical Modeling of Saturated and CO_2 Sequestration Systems

The fourth day will be focused on geochemical modeling using the Equilibrium, Conservation, Kinetic, Equation Chemistry (ECKEChem) module (White and Fang, 2012) for the simulator. The day will start with an overview lecture on the ECKEChem module, covering its mathematical formulation, numerical solution scheme, implementation in the code, and required inputs. Three types of geochemical problems will be considered. The first problem will involve species transport and reactions for a mixed geochemical and micro-biological system. The second problem will involve the transformation of a glauconitic sandstone formation with the injection of CO_2. The third problem will contrast these mineralization reactions with those for a basaltic reservoir. The increased complexity of the input files for geochemical modeling warrants a full day of instruction during the short course. The number of problems addressed will depend on the students' pace. The day will close with a student workshop where students will be free to work on unfinished problems or explore new problems of their own. The course instructors will be available during the workshop for mentoring.

※ White M. D., and Y. Fang. 2012. "STOMP-ECKEChem: An Engineering Perspective on Reactive Transport in Geologic Media." In *Groundwater Reactive Transport Models*, pp. 112-140. Bentham eBooks, DOI: 10.2174/97816080530631120101, eISBN: 978-1-60805-306-3.

- ECKEChem Overview Lecture
- ECKEChem Preprocessors
- ECKEChem Input
- Reactive Transport Problems
- Participants' Workshop
- Transport, Kinetic Biodegradation, Cell Growth and Sorption : This example problem was developed and published by Parkhurst and Appelo (1999), from an advective-dispersive-reactive transport problem, developed by Tebes-Steven and Valocchi (1998). The transport involves mobile and immobile species where the immobile species are either bacterial cells or sorbed metals. The chemistry involves speciation, bacterially mediated degradation of an organic substrate, bacterial growth and decay, and kinetic metal sorption, including metal-ligand complexation. In brief, the problem involves the steady-flow of an aqueous solution through a 10-m column, initially containing biomass. A pulse of dissolved nitrylotriacetate (Nta) and cobalt (Co) are introduced at the inlet of the column. Nta is defined to degrade in the presence of biomass and oxygen, yielding biomass growth. The equilibrium chemistry in this problem assumes activity coefficients of 1.0.

※ Parkhurst, D. L. and C. A. J. Appelo. 1999. *User's Guide to PHREEQC (Version 2) – A Computer Program for Speciation, Batch Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations*, Water-Resources Investigation Report 99-4259, U.S. Geological Survey.

※ Tebes-Steven, C. and A. J. Valocchi, J. M. van Briesen, and B. E. Rittmann. 1998. "Multicomponent transport with coupled geochemical and microbiological reactions –model description and example simulations." *Journal of Hydrology*, 209:8-26.

- Mineral Trapping in a Glauconitic Sandstone Aquifer (GeoSeq #5) : This problem addresses geochemical effects of CO_2 injection into a glauconitic sandstone aquifer and analyses the impact of CO_2 immobilization through carbonate precipitation. This problem is based on Problem 5 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002). Batch reaction modeling of the geochemical evolution of this aquifer is performed in the presence of CO_2 at high pressure. The problem is based on Gunter et al. (1997), who modeled water-rock reactions when CO_2 is injected into a glauconitic sandstone aquifer in the Alberta Sedimentary Basin, Canada.

※ Gunter W.D., B. Wiwchar, and E.H. Perkins. 1997. "Aquifer disposal of CO2-rich greenhouse gases: Extension of the time scale of experiment for CO2-sequestering reactions by geochemical modelling." *Mineralogy and Petrology*, 59(1-2):121-140.
Pruess, K., and J. Garcia. 2002. "Multiphase flow dynamics during CO2 injection into saline aquifers." *Environmental Geology*, 42:282-295.

- Mineral Trapping in a Basaltic Formation : Continental flood basalts represent one of the largest geologic structures on the planet but have received comparatively little attention for geologic storage of CO_2. This problem is based on Bacon et al. (2011), who investigated the injection of CO_2 into the Columbia River Basalt formation and its subsequence reaction with the basalt minerals. The problem involves the injection of a pilot-scale amount of CO_2 into three basalt flow tops, which have high intrinsic permeability, compared with the intervening flow interiors with relatively low intrinsic permeability. The coupled well model is used to inject 1000 tonnes of $scCO_2$ over a 14-day period. The simulation considers geochemical reactions involving the minerals present in the formation, the formation brine, and injected supercritical CO_2. After the injection of supercritical CO_2, CO_2 dissolves into the aqueous phase, up to the equilibrium solubility limit. Aqueous CO_2 dissociates into bicarbonate and carbonate ions, producing H+ and lowering the pH. The pH of the residual formation water in contact with the injected CO_2 decreases from an initial value of 9.6 to values as low as 4 just after injection. The lowered pH drives the dissolution of primary minerals in the basalt, producing Ca+, Mg+ and Fe+ which combine with the aqueous CO_2 to form carbonate secondary minerals. After 13 years, 25% of the injected CO_2 has dissolved and 25% has precipitated as carbonate minerals.

※ Bacon D.H., H.T. Schaef, and B.P. McGrail. 2011. "Field-Scale Simulation of CO_2 Sequestration in Columbia River Basalt." In Proceedings of Tenth Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA on May 4, 2011. PNWD-SA-9378.

- ## Day 5. Viscous Fingering of Dissolved CO_2 and Geomechanical Modeling of Geologic Sequestration Systems

The final day will have a split focus. During the morning the focus will be on the geomechanical response to the injection of CO_2 into a deep saline reservoir. This focus will open with an overview lecture on the Elastic-Plastic Mechanical (EPMech) module for the simulator, which uses the RIEM (Rigid-Body Interface Element Method) for geomechanical modeling. The geomechanical focus will continue with the students working through a geomechanical problem that investigates surface deformation that occurs in response to geologic sequestration of CO_2. The second focus for the final day will be on viscous fingering that occurs in response to CO_2 saturated brine overlying CO_2 unsaturated brine in a porous media. The participants will investigate scale effects and the triggering of viscous finger formation. The day will close with participants' workshop where students will be free to work on unfinished problems or explore new problems of their own. The module instructors will be available during the workshop for mentoring.

- EPMech Overview Lecture
- EPMech Input
- Geomechanical and Viscous Fingering Problems
- STOMP-EOR Overview and Demonstration
- Participants' Workshop
- Caprock Hydromechanical Changes Associated with CO_2 Injection into a Brine Formation : This problem is based on the study of hydromechanical changes predicted to occur with the injection of supercritical CO_2 ($scCO_2$) into a deep saline formation, published by Rutqvist and Tsang (2002). Instead of coupling STOMP with a commercial geomechanical simulator, however, the problem is solved with STOMP-CO2 and the EPMech module, yielding an integrated solution package. The problem involves injecting $scCO_2$ at a constant rate over a 10-year period into a 200-m thick reservoir, with a 100-m thick caprock. The reservoir-caprock interface is assumed to be horizontal at a depth of 1300 m. The hydraulic and mechanical responses to the injection are predicted by the simulation.

※ Rutqvist J. and C.-F. Tsang. A Study of Caprock Hydromechanical Changes Associated with CO_2 Injection into a Brine Aquifer, *Environmental Geology*, Vol. 42, pp. 296 - 305, 2002.

- Viscous Fingering with Dissolution of CO_2 into Brine : This problem investigates the modeling of viscous fingering that results when CO_2 dissolves into brine creating an unstable fluid density condition (i.e., higher density fluid over a lower density fluid). Two different scenarios are considered: 1) injection of CO_2 into a laboratory-scale two-dimensional flow cell filled with accusands, and 2) dissolution of CO_2 at the top of a two-dimensional Hele-Shaw cell, filled with micro-beads. In both simulations the higher density of the CO_2-saturated brine above the CO_2 free-brine leads to gravitational instability and consequently convective fingers appear in minutes. Simulations will be conducted with variations in permeability and flow cell dimensions to vary the characteristic Rayleigh number. The participants will additionally investigate methods for altering the induction time through heterogeneities in permeability, grid resolution, and initial conditions.

About the instructor – (Module 1) Dr. Timothy Scheibe

Dr. Timothy Scheibe is a Senior Research Scientist in the Hydrology Group at the Pacific Northwest National Laboratory. He received a Bachelor's degree in Geological Engineering from Washington State University, a Master's in Civil Engineering from the University of Washington, and a Ph.D. in Civil Engineering from Stanford University. His research focuses on numerical simulation of biogeochemically reactive transport in subsurface aquifers and reservoirs, applied to a variety of problems including microbial transport in groundwater, carbon sequestration in soils and the deep subsurface, and bioremediation of metals and radionuclides. He is currently collaborating with computational scientists, microbiologists and geochemists to simulate coupled flow, transport, and biogeochemical processes at cellular, pore and continuum scales using high-performance computational resources. He is the focus area lead for numerical model development efforts under PNNL's Microbial Communities Initiative and Carbon Sequestration Initiative, and is leading an effort to benchmark numerical models for simulation of Enhanced Geothermal Systems. Dr. Scheibe currently serves on the editorial board of the journal *Ground Water* (since 2001) and is active in several scientific societies including the American Geophysical Union, in which he is a member and former chair of the Groundwater Technical Committee. He has approximately 50 peer-reviewed publications in ISI-indexed scientific journals (http://www.researcherid.com/rid/A-8788-2008). He is frequently invited to lecture at conferences and universities, and in 2010 he served as the Henry Darcy Distinguished Lecturer (sponsored by the National Ground Water Association), in which capacity he gave 65 invited lectures nationally and internationally.

About the instructor – (Module 2) Dr. Charlotte Sullivan

Dr. Charlotte Sullivan is a Senior Research Scientist in the Geosciences Group of the Energy and Environment Division at the Pacific Northwest National Laboratory. She received a Bachelor's degree in Geology from Arkansas Tech University, a Master's in Geology with a thesis on stratigraphy from the University of Arkansas, and a Ph.D. in Geology from the University of Houston with a dissertation on numerical analysis of sedimentary constituents of reefs in the Philippines and Indonesia.

Dr. Sullivan's technical expertise is in subsurface geology with over 30 years in research, exploration and production in the petroleum industry, and in academia; with special emphasis on sequence stratigraphy, reservoir characterization, and calibration of seismic attributes. Dr. Sullivan has lived and conducted geological work in Singapore, Jakarta, and Manila, and has worked on subsurface characterization of hydrocarbon reservoirs in Mexico, Qatar, and major basins of the U.S. Dr. Sullivan was a strategic hire for PNNL in December 2005 to bring advanced petroleum-industry reservoir characterization and geophysical technologies to subsurface research efforts. Although most of her current projects are focused on developing applied geophysical/geological research programs related to selection, operation, monitoring, and risk management of the geologic sequestration of carbon dioxide in sedimentary rocks and basalt, she is also involved in geophysical research on unconventional hydrocarbon resources, and enhanced oil recovery, especially in carbonate and fractured reservoirs.

Dr. Sullivan taught Petroleum Geology at the University of Houston, and industry short courses related to petroleum geology and subsurface imaging. At PNNL she has taught short courses on geologic sequestration of anthropogenic carbon dioxide, and frequently presents results of current research at regional, national and international venues. Her publications include carbonate sedimentology, seismic attributes, and reservoir characterization of hydrocarbon reservoirs and carbon storage reservoirs.

Dr. Sullivan is a past member of the Indonesian Petroleum Association, and is a current member of the American Association of Petroleum Geologists, and the international Society of Exploration Geophysicists. She is also an active member in a number of regional professional geologic societies

About the instructor – (Module 3) Dr. Mark White

Dr. Mark White, a Senior Research Engineer in the Hydrology Group at the Pacific Northwest National Laboratory, is the principal author of the U.S. Department of Energy supported multifluid subsurface flow and reactive transport simulators STOMP and eSTOMP. STOMP is a sequential scientific computer code that comprises a collection of operational modes for modeling multifluid flow and reactive transport through variably saturated geologic media. eSTOMP is a scalable, parallel scientific computer code, which like STOMP, comprises a collection of operational modes for modeling subsurface flow and reactive transport and is being implemented on the massively parallel computers at the Environmental Molecular Science Laboratory. eSTOMP is currently under development, offering a subset of the STOMP operational modes and process modeling capabilities. The STOMP and eSTOMP simulators are currently being used nationally and internationally at research laboratories and universities. Additional information about the STOMP simulator is available via the internet (http://stomp.pnnl.gov).

About the instructor – (Module 3) Ms. Signe White

MS. Signe White, a Senior Research Scientist in the Environmental Characterization and Risk Assessment Group at the Pacific Northwest National Laboratory, has over 20 years of experience in subsurface flow and transport modeling. Ms. White is a member of the STOMP development team, the STOMP short-course instructional team, the website content team, and the development team for the Geologic Sequestration Software Suite (GS^3), a software framework for collaborative carbon sequestration modeling. The GS^3 framework is currently being used on the U.S. Department of Energy (DOE) sequestration projects SimSeq and FutureGen 2.0. Ms. White is the lead numericist for the FutureGen 2.0 project and Arches geologic sequestration projects at PNNL. The FutureGen 2.0 Project is a first-of-a-kind, near-zero emissions, coal-fueled power plant, being developed in cooperation with the U.S. DOE; where a power plant in Meredosia, Illinois is being upgraded with oxy-combustion technology to capture 1.3 million tonnes of CO_2 each year. Ms. White received the 2002 Fitzner-Eberhardt Award for outstanding contributions to science and engineering education, and the 2004 PNNL Woman of Achievement Award.

Korea Institute of Geoscience and Mineral Resources

GENERAL INFORMATION

- **STARTING/END DATE AND LOCATION**
  - November 4 – November 15 (2 weeks) at KIGAM in Daejeon, Korea.

- **LANGUAGE OF STUDY**
  - The language of instruction is English and all courseware is in English.

- **ASSESSMENT AND CERTIFICATION**
  - Participants will receive certificates upon completion of the course.

- **REGISTRATION**
  - **Deadline** – Participants should fill in the application from and send it to E-mail below
    - By October 11 for a nominee
    - Before 7 days in starting date of each module for someone else except for a nominee
  - **How to Register**
    - Complete and return the attached form, **"Nomination form"** for a nominee and "Application form" for someone else except for a nominee to Mr. Seung-Ryeol Hwang (hwang3816@kigam.re.kr by email
    - Visit at http://isgeo.kigam.re.kr, IS-Geo URL. You can learn more about all training courses in IS-Geo website.

- **COURSE FEE**
  - The fee for each module contains the course notes, the certificate of attendance and the Pre-Course e-Learning.
  - **The fee for a nominee is free.**
  - The fee to someone else except for a nominee in each module is 500,000 Korean Won / Module (100,000 Korean Won /Module for only students).

- **CONTACT**
  - For more inquires about training courses of IS-Geo, please contact at any time
  - **Mr. Seung-Ryeol Hwang** (hwang3816@kigam.re.kr) by email or by phone at +82-(0)42-868-3816.