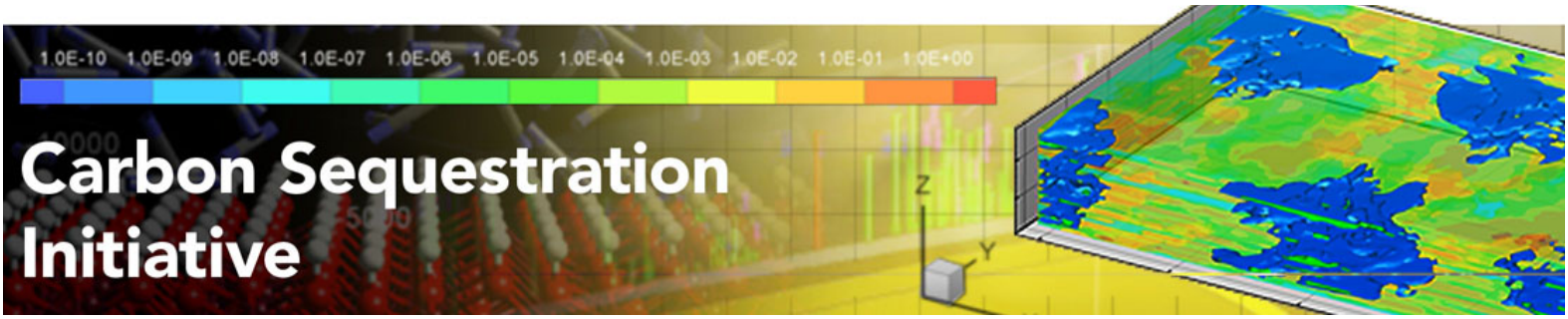

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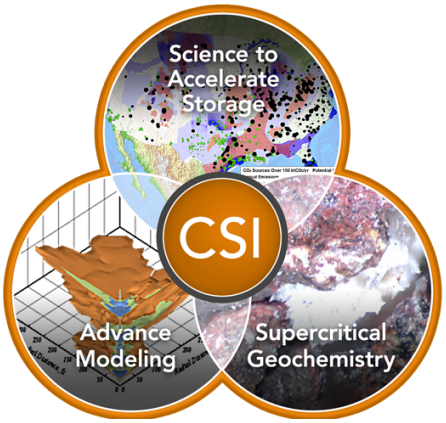
Carbon Sequestration Initiative

The Carbon Sequestration Initiative (CSI) is a 5-year, multi-million dollar investment to advance PNNL's capabilities in geologic sequestration. This initiative will enable the rapid and safe deployment of geologic emissions storage with new tools to advance our scientific understanding of geologic sequestration processes and facilitate the incorporation of these advances into scientific simulators. CSI researchers are developing a computational environment (Geologic Sequestration Software Suite or GS^3) and an experimental suite (In Situ Supercritical Suite or IS^3) that promotes research collaborations to accelerate the pace of scientific discovery.

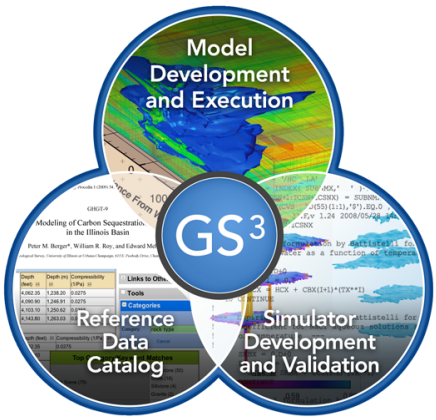


The initiative is developing new experimental techniques for understanding mechanisms of mineral dissolution and carbonate precipitation for both aqueous and supercritical carbon dioxide phases under in situ conditions. The initiative is also developing innovative software to manage data, simulate storage projects, and automatically benchmark simulators. This computational platform will enable national and international research collaborations to validate new science in the simulators. In addition, GS^3 provides accessibility of the most advanced scientific simulators to domain users for application to field sites. Initially, the tools developed under this initiative can be used to facilitate collaborations among the DOE Regional Carbon Sequestration Partnerships and collaborative R&D with China.

The initiative projects are managed under two focus areas, GS^3 and IS^3, which are described below.

Geologic Sequestration Software Suite

The Geologic Sequestration Software Suite, GS^3, is an extensible, dynamic and integrated computing environment that stewards the data, scientific software, analytical tools, and computing resources. This framework is designed to reduce modeling process burdens on scientists and engineers by encouraging interdisciplinary teams, making computational tools more accessible, and automatically tracking data provenance.



GS^3 is currently under development. Principal development objectives are to create a dynamic and collaborative environment with mechanisms to control access, provide a non-proscriptive approach to the modeling process, establish a current suite of scientific simulators and development and analytic tools, and use existing open source software for the framework.

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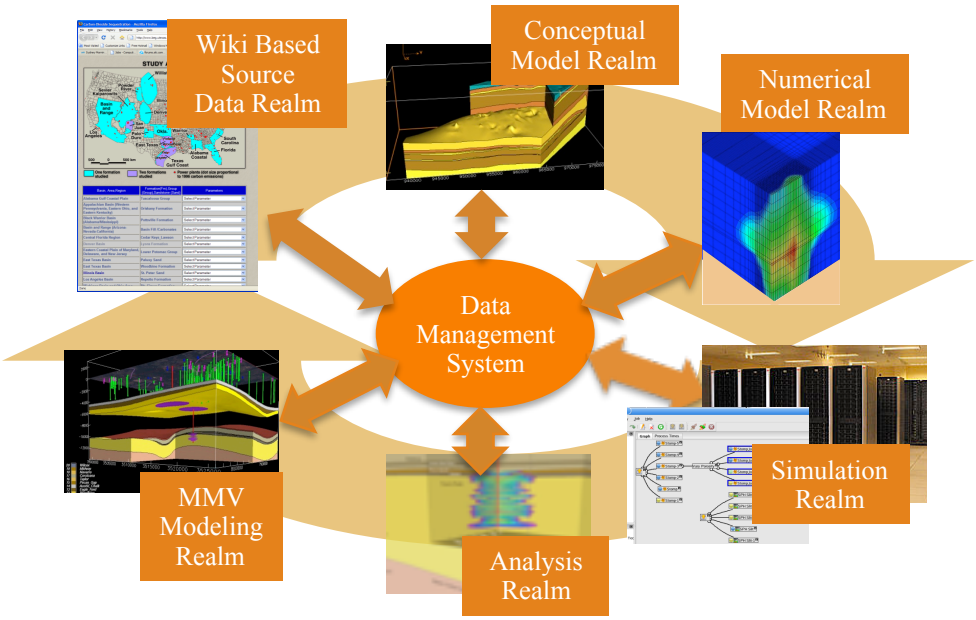
A typical workflow for the modeling process is shown in the figure below. This computational framework provides scientists and engineers with flexibility in their approach to geologic sequestration modeling, affording them a wealth of scientific tools and data never before realized. GS^3 keeps track of data input from different team members working on the same site and tracks models through the simulations process. GS^3 is web-based, so team members can collaborate regardless of their geographic location.



GS^3 is designed for two user communities, application engineers, who may be modeling a specific site for geologic sequestration and development engineers, who want to advance the scientific simulators. Application engineers will have access to the most current open-source scientific simulators and computational tools, and developers will have a platform to quickly validate changes and improvements incorporated into the scientific simulators. As the geologic sequestration technology matures through laboratory experiments and field demonstrations, GS^3 will provide a platform for benchmarking scientific simulators and new theoretical ideas against recognized standards. The vision is for GS^3 to serve as a platform for an eventual community based subsurface model for geologic sequestration.

GS^3 Projects

Geological Sequestration Software Suite Core Architecture and Simulation Framework
PIs: Ian Gorton, Gary Black, Karen Schuchardt, Signe Wurstner

The Geological Sequestration Software Suite (GS^3) framework incorporates off-the-shelf tools that many modelers are already familiar with; facilitates the creation/integration of custom tools, utilities, and scripts; and integrates seamlessly with data management capabilities including provenance capture and user annotation. In addition to the component integration framework, this project will provide the data management services, standardized formats, data translations, and automated computational job management. Ultimately, the GS^3 framework will vastly reduce the burden on modelers for manually organizing and tracking the volumes of data and applying the variety of tools needed throughout the sequestration modeling lifecycle.

Geologic Sequestration Software Suite: Data Assimilation Tools for CO_2 Reservoir Model Development
PIs: Mark Rockhold, Chris Murray, E. Charlotte Sullivan, Gary Black

This project is developing focused computational tools that allow scientists and engineers to efficiently assemble, assimilate, and track large volumes of disparate data for building geologic models of CO_2 sequestration. Open-source and PNNL-developed reservoir characterization and visualization software tools will be available through GS^3 for data assimilation and conceptual-mathematical model building in support of carbon sequestration modeling.

Geologic Sequestration Software Suite: Numerical Model Development
PIs: Mark Williams, Signe Wurstner, Paul Thorne, Andrew Kuprat, Diana Bacon

This project addresses the need for numerical model development tools and innovative methods to support the generation of simulator input files as part of the Geologic Sequestration Software Suite (GS^3). These algorithms and tools will improve translation of conceptual models to the numerical framework required by simulators (e.g., STOMP, PFLOTRAN, TOUGH2, FEHM) and provide the capability of generating multi-scale (spatial and temporal) numerical models to support the operational and long-term performance simulation needs for geologic sequestration technology.

Geologic Sequestration Software Suite: Benchmarking and Validation Platform
PIs: Mark White and Peter Hui

This project is producing a benchmarking and validation platform for accelerating the development and enhancement of numerical simulators for carbon sequestration. The platform will contain 1) an evolving suite of validation problems for geologic sequestration that define the state of numerical simulation science, 2) a software configuration and control program to promote the advancement of numerical simulation science, and 3) a computational environment that encourages the development of a national community simulator for geologic sequestration. A critical component of this project will be the involvement of the geologic sequestration community in the initial development of validation problems.

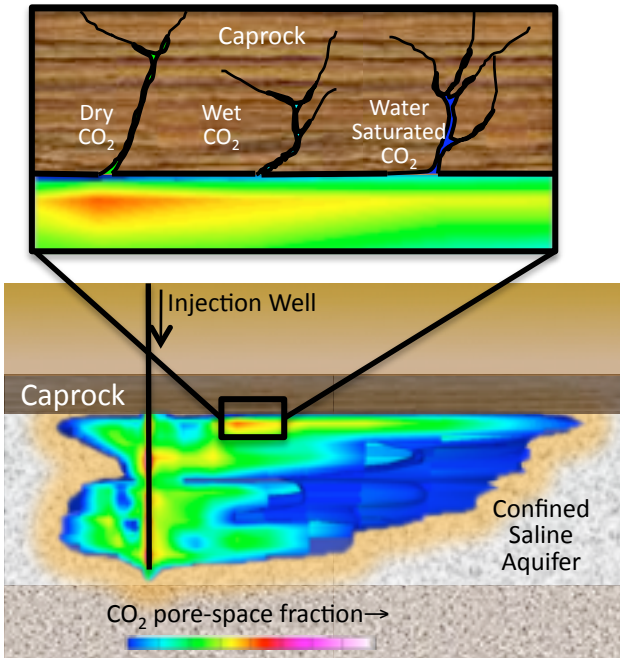
Multiscale Investigation of CO_2 Behavior in Subsurface Under Extreme Conditions
PIs: Alexandre Tartakovsky, Andres Marquez, Sebastien Kerisit, Guang Lin

This project is developing multiscale multiphase flow and transport models to simulate CO_2 behavior (flow and precipitation) in the caprock at the pore and sub-pore scales. This hybrid model will be able to bridge molecular dynamics (MD) surface chemistry models and pore-scale models and will be able to describe the complex behavior of CO_2 in the subsurface in general and in the caprock, specifically. The hybrid model will serve as a basis for the upscaling of the CO_2 behavior from the fundamental scales to the scale of practical importance. Reactions at the fundamental scale are currently being performed in the IS^3 focus area of this initiative and are planned in new Energy Frontier Research Centers funded by Basic Energy Sciences.

In Situ Supercritical Suite

The In Situ Supercritical Suite or IS^3 is a group of one-of-a-kind instruments that will allow researchers to probe geochemical reactions under supercritical pressures and temperatures. Instrumentation at the Environmental Molecular Sciences Laboratory (EMSL) at PNNL is being modified for high pressure and temperature sequestration experiments. The focus of the experiments is to understand supercritical geochemistry of the caprock and injection and monitoring boreholes.

It has been found that CO_2 dissolved in groundwater in deep saline aquifers has minimal reaction with the mineral matrix of the reservoir. It has also been found that pumping supercritical CO_2 into a reservoir has a drying affect around the borehole. This is illustrated in the cross-section below of supercritical CO_2 injected into a saline aquifer.



Current simulators represent reactions where CO_2 is first dissolved in water, so thermodynamic and kinetic parameters are valid as long as water is the solvating fluid. Research at PNNL has shown that when CO_2 is the solvating fluid and contains small amounts of water, this solution is highly reactive with minerals. In addition, CO_2 trapping processes over the short-term (e.g., capillary trapping) and long-term (e.g., mineralization) depend on how the chemistry of the fluid-mineral interfaces evolves over time. The rate and extent of reaction at fluid-mineral interfaces around the injection borehole and at the caprock are important scientific unknowns that must be resolved.

The cross-section also illustrates the buoyancy of supercritical CO_2 and therefore the importance of the caprock. Integrity of the caprock will determine the long-term permanence of CO_2 storage in deep geologic reservoirs. Therefore, understanding fracture opening or self-sealing in the caprock is critical.

IS^3 Projects

In Situ Nuclear Magnetic Resonance Investigations of Trapping Mechanisms in CO_2 Storage
PIs: David Hoyt, Jianzhi Hu, Ja Hun Kwak, Jesse Sears

This project is developing a unique in situ magic angle spinning NMR instrument capable of supercritical CO_2 conditions for study of mineral reaction mechanisms and kinetics. This capability will provide new fundamental insights into the molecular mechanisms of mineral interfacial reactions with CO_2, the effects of small amounts of dissolved water on this reaction, the effects of structural and chemical heterogeneity at the interfaces on the reaction kinetics, and the macroscopic dynamics of CO_2 and water at relevant geological temperature and pressure.

Development of a Real-Time Optical Spectroscopy Platform for Molecular-Level Investigation of Mineral Transformation in Supercritical Carbon Dioxide
PIs: Zheming Wang, Chris Thompson, Alan Joly

This project will result in new and unique research capabilities for performing optical spectroscopic studies of mineral carbonation processes involved in sequestration, from mineral dissolution/nucleation/precipitation and hydration/dehydration, to in situ sorption/desorption studies in supercritical CO_2 with variable amounts of water present. This project will develop a novel pressurized optical cell flexible enough for a range of complementary measurements including infrared absorption spectroscopy, Raman spectroscopy, fluorescence spectroscopy, and nonlinear optical methods.

In situ Imaging of Mineral-Supercritical CO_2 Reactions with Atomic Force Microscopy
PIs: Scott Lea, Steve Higgins (Wright State), and Jim Amonette

This project is developing a one of a kind microscopy capability to investigate dissolution and growth processes of mineral surfaces in contact with supercritical CO_2 at the molecular scale. This atomic force microscope will be the first that is capable of operating at supercritical CO_2 conditions. It will be able to operate in both CO_2-dominant and water dominant supercritical CO_2-water phases where mineralization, dehydration, and chemical changes in mineral wettability occur.

In Situ High-Pressure XRD Investigation of Caprock Mineral Reactions with Water Solvated in Supercritical CO_2
PIs: H. Todd Schaef and Ken Krupka

This project will develop an x-ray diffraction capability in which mineral transformation reactions induced by contact with supercritical CO_2 bearing variable amounts of water can be detected in situ. This capability will allow the study of mineralogy changes in real-time and with mineral specificity for bulk transformations at the pore-scale.

Micromodel Pore-Scale Studies of Caprock-Sealing Efficiency and Trapping Mechanisms Related to CO_2 Sequestration
PIs: Mart Oostrom, Jay Grate, Changyong Zhang, and S.K. Sundaram

This project will develop a one of a kind high-pressure microfluidics capability to investigate pore-scale reactive transport phenomena that play a direct role in the potential for leakage from deep aquifers/reservoirs through the caprock, and the storage capacity of injection sites by hydrodynamic (primary) and capillary (secondary) entrapment. Highly precise micromodels will be produced along with capabilities for directly imaging displacement processes, fluid mixing and compositional gradients, and capillarity.