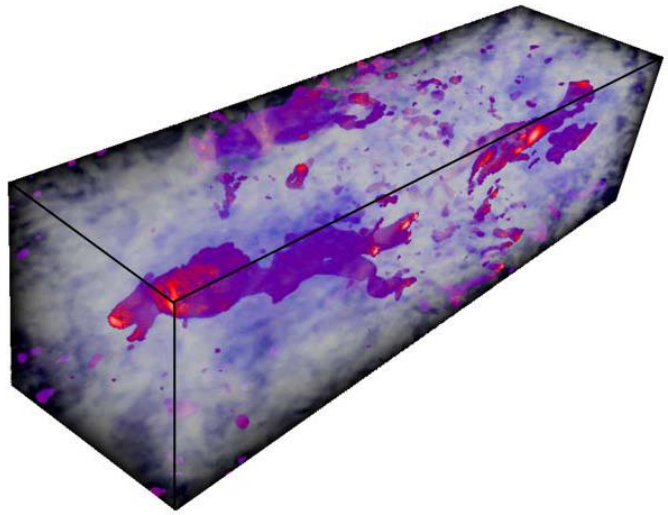
An integrated experimental and numerical study: Developing a reaction transport model that couples chemical reactions of mineral dissolution/precipitation with spatial and temporal flow variations in CO_2/brine/rock systems



Lattice-Boltzmann simulation of gas flow through a porous medium (red indicates high speeds).

PI: Martin Saar

University of Minnesota

Track: Chemistry, Reservoir and Integrated Models

May 20, 2010

Mandatory Overview Slide

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Timeline:	Project start date:	01/08/2010 (effective start: 04/01/2010)
	Project end date:	02/28/2013
	Percent complete:	~0-2%
Budget:	Total:	$1,937,523.00
	DOE share:	$1,550,018.00
	Awardee share:	$ 387,505.00

Relevance/Impact of Research

Project Outcome: This project will result in a numerical simulator (modified version of TOUGH2) that can adjust porosity and permeability fields according to experimentally observed chemical fluid-rock interactions (mineral dissolution or precipitation) under realistic conditions likely found when supercritical CO_2 is injected into geothermal reservoirs for heat energy extraction.

Relevance: The simulator can thus help determine if CO_2 injection into EGS brines will cause clogging of pore spaces or dissolution of host rocks with potentially detrimental consequences to heat extraction. As a result, this simulator will play a critical role when assessing long-term sustainability of geothermal energy utilization in enhanced and natural geothermal systems. The simulator can also be used to evaluate long-term CO_2 sequestration potentials.

Relevance/Impact of Research

Objectives:

1) Generate and characterize mineral dissolution/precipitation reactions in supercritical CO_2/brine/rock systems under pressure-temperature-chemistry conditions resembling CO_2 injection into EGS.
2) Characterize three-dimensional spatial and temporal distributions of rock structures subject to mineral dissolution/precipitation processes by X-ray tomography, SEM imaging, and Microprobe analysis.
3) Obtain spatial and temporal fluid velocity distributions in transient non-reacting multi-fluid flows through porous media to test and qualify Lattice-Boltzmann simulators (see Objective 4).
4) Develop Lattice-Boltzmann (LB) multiphase-multicomponent fluid flow simulators that include temporal and spatial variability as well as chemical reaction capability to allow detailed accurate numerical modeling of chemical fluid-mineral/rock interactions in complex pore, fracture, and conduit openings.
5) Employ results from previous four objectives to develop parameterized equations for permeability changes (as a function of temperature, pressure, chemistry, time, heterogeneity) and integrate them into TOUGH2.

Tasks to be performed:

1) **Laboratory experiments with supercritical CO_2, brine, rock:**

   We propose to conduct laboratory studies of interactions between supercritical CO_2, water and/or brine, and end-member rock types (arkose sandstone and basalt) selected from likely CO_2 injection sites using state of the art experimental and analytical facilities.

2) **X-ray tomography and other methods to characterize 3D rock matrix structures:**

   At various stages of the reaction experiments (Task 1.0), the three-dimensional (3D) geometry of the pore space will be analyzed in a non-destructive manner by high-resolution (sub-micron) X-ray tomography scanning providing a novel approach to constrain better the specific locations of mineral dissolution and precipitation over time.

3) **PIV measurements of multi-fluid, non-reacting flows through porous media:**

   Particle image velocimetry (PIV) will be employed to obtain spatial and temporal fluid velocity distributions in transient non-reacting multi-fluid flows through a transparent porous matrix.

4) **Development of a new approach for reactive transport modeling:**

   Implementation and validation of a LB code that incorporates both physical and chemical effects inherent to the injection and flow of supercritical CO2 through brine/rock systems. The non-reacting version of the code will be validated against the results obtained in Task 3.0. Time series 3D X-ray scans from Task 2.0 will be used as input to the more sophisticated LB code that includes dissolution/precipitation effects.

Tasks to be performed (continued):

5) Development of a new approach for reactive transport modeling:

A tested and validated (Task 3.0) LB-method simulator (Task 4.0) would allow more robust simulations of fluid and solute flow through the X-ray-generated 3D representations (Task 2.0) of the experimentally modified (Task 1.0) pore spaces, including simulations of reactions and related pore space geometry modifications.

The changes in pore space geometry over time can then be compared to the time series of X-ray images from actual experiments. A time series representation of 3D pore space (i.e., rock distribution) and fluid component/phase data would be achieved for the experimental *P*, *T*, chemistry conditions.

Thus, the relationship between fluids, rocks, and physical/chemical conditions and the resultant pore space geometry (pore connectivity, porosity, tortuosity, specific surface area) can be deter-mined and parameterized.

While this parameterization is empirical, it is specifically not based on traditional chemical reaction rate laws (which are inadequate for the usually complex chemical and physical conditions with which we are concerned). Hence, results will represent a paradigm shift in describing pore space, and thus permeability, modifications during fluid-mineral interaction. The final stage in our integrated experimental and numerical approach is to incorporate the parameterized fluid-rock interaction rules into TOUGH2 to allow for large-scale simulations of fluid flow with associated reactions applicable to chemical and physical processes in natural systems and laboratory simulations of these systems.

Accomplishments, Expected Outcomes and Progress

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Team qualification:

Dr. Martin Saar (PI):

Fluid dynamics simulations in the geosciences with particular emphasis on lattice-Boltzmann and TOUGH2 simulations.

Dr. William Seyfried, Jr. (co-PI):

Aqueous geochemist → will conduct laboratory experiments.

Dr. Ellen Longmire (co-PI):

Particle Image Velocimetry experiments to test LB code.

Project Management/Coordination

Timeline for Project-Related Tasks

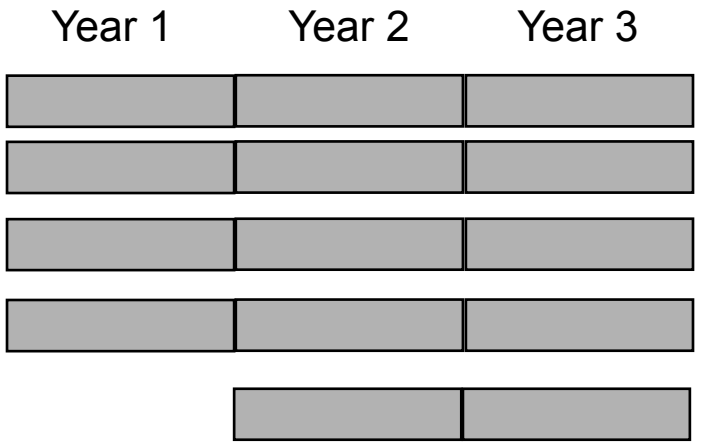
Task 1: CO_2 injection experiments

Task 2: Solid characterization

Task 3: PIV on multiphase flow through porous media

Task 4: LB code development

Task 5: TOUGH2 modification



For specific task accomplishments, see previous slides.

This project does not include key milestones or go/no-go decision points as tasks occur concurrently.

Future Directions

All of previous presentation is future work as the project just started.

Mandatory Summary Slide

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