



Development of Chemical Model to Predict the Interactions between Supercritical CO₂ and Fluid, and Rocks in EGS Reservoirs

Chuan Lu

University of Utah

- **Project Timeline**

03/31/2010—04/30/2013, 3% completed

- **Budget**

Total project funding \$1,384,213, DOE share \$944,707, awardee share \$441,507, funding received in FY09 \$0, funding for FY10 \$311,859 (DOE share)

- **Barriers (Y)**

Existing models have limitations (the pressure and temperature ranges are limited) and cannot sufficiently address all of the GTP analytical needs and requirements (pressure up to 100 MPa, temperature up to 300° C)

- **Partners**

- AltaRock Energy, INC.
- Los Alamos National Laboratory
- University of Wyoming

Develop a chemical model, based on existing models and databases, that is capable of simulating chemical reactions between supercritical (SC) CO₂ and Enhanced Geothermal System (EGS) reservoir rocks of various compositions in aqueous, non-aqueous and 2-phase environments. The specific objectives include:

- Build thermodynamic database over P-T range relevant to EGS
- Estimate feasible chemical reactions and corresponding rate constants
- Extend reactive-transport models to EGS
- Investigate the interactions of CO₂ and reservoir rocks
- Conduct numerical experiments on idealized EGS, including reservoirs and surface facilities

The project directly addresses several critical needs of developing EGS using CO₂ as a working fluid. The methods and models developed in the scope of work will take into consideration dominant chemical reactions, kinetics, risk, and feasibility including the coupling of EGS development concurrent with geologic carbon dioxide sequestration.

- Build the thermodynamic database (M1) (12/31/2010)
 - Databases will be assembled and/or updated for thermodynamic and kinetic rate laws for water/brine/rock/CO₂ interactions at the P and T conditions common to EGS.
 - Reference datasets include EQ3/6, Phreeqcl, SOLTHERM databases and sprons96, slop98 for SUPCRT92 software.
 - The methodology adapted to expand the reaction equilibrium to high P, T conditions is similar to that used by SUPCRT92.
- Develop the reactive-transport model (12/31/2011)
 - Thermodynamic analysis will be conducted to determine applicable chemical reactions. (M2)
 - Existing open source subsurface reactive flow and transport simulators (TOUGHREACT and PFLOTRAN) will be modified. (M3)
 - TOUGH family codes have been widely used in modeling EGS and CCS processes. The fracture-matrix feature can be handled through the MINC module; however, at considerable cost.
 - With a new thermodynamic database and future development of dual-continuum capability, the massively parallel features of PFLOTRAN (run on 2¹⁷ processors with 2 billion grid cells) can facilitate simulations with high-resolution, large domain size and multiple realizations.
- Model calibration and verification (End of project)
 - We will collect data from literature, extrapolate existing data and conduct experimental laboratory work to calibrate and verify the datasets
 - Experiments and simulations will follow an iterative process in which experimental results are interpreted with geochemical codes (GWB, TOUGHREACT and/or PFLOTRAN) and computational results are used to aid the design of subsequent experiments.
 - Kinetic rate constants will be estimated during this process. (M4)

- Numerical simulations to investigate (End of project)
 - the interactions between injected SC CO₂ and EGS reservoir fluids and rocks (in fractures, matrix and integrated systems) (M5)
 - the possibilities and suitable conditions of using CO₂ as a working fluid (sensitivities on reservoir and operation conditions), as an acidization agent (calcite in fractures), and the simultaneous operation of CO₂ geologic storage (reopening of far reaching fractures and faults) (M6)
 - mineral and salt precipitation in production wells and surface equipments (1D simulations for production wellbore, pipeline and heat exchanger, thermodynamic analysis on turbines) (M7)
- Go/No-Go decision (12/31/2011)

The accomplishment of the code modifications and the successful development of the new database, will provide essential tools to evaluate the interactions between SC/dissolved CO₂ with reservoir rocks for aqueous, two phase and anhydrous conditions in EGS reservoirs. The no-go decision will be made if one of the following scenarios occurs:

 1. the new database and thermodynamic analyses cannot be completed because of lack of critical data necessary for performing EGS simulations;
 2. an explicit fracture model or the dual continuum model combined with chemical reactions is computationally too demanding to carry out practical calculations for an EGS.

- Program initiation
 - Select minerals and aqueous species to be included in the database(LANL,UU)
 - Design experiment (UW)
 - Recruit post-doctoral research assistant (LANL) and graduate students (UU and UW)
- Planned outcomes
 - The thermodynamic database containing key mineral and aqueous species in EGS at elevated pressure (up to 100MPa) and temperature (up to 300° C)
 - Estimations on thermodynamic feasible reactions and kinetic rate constants

(by Dr. Lu Dr. Han Dr. Moore and Dr. Rose at UU, Dr. Lichtner at LANL, Dr. Larson at AltaRock, Dr. Kaszuba at UW)

 - Model calibration and verification with experimental work (experimental work will be conducted by Dr. Kaszuba at UW.)

- **Planned outcomes (cont.)**

- Open source reactive-transport model and simulators (by Dr. Lu at UU and Dr. Lichtner at LANL)
- Investigations of interactions between supercritical CO₂ and reservoir rocks under aqueous, anhydrous and two-phase conditions
- Evaluation of conditions suitable for using CO₂ as working fluid, as acidization agent, and the possibility of concurrent carbon sequestration
- Investigations on mineral precipitation in EGS surface facilities

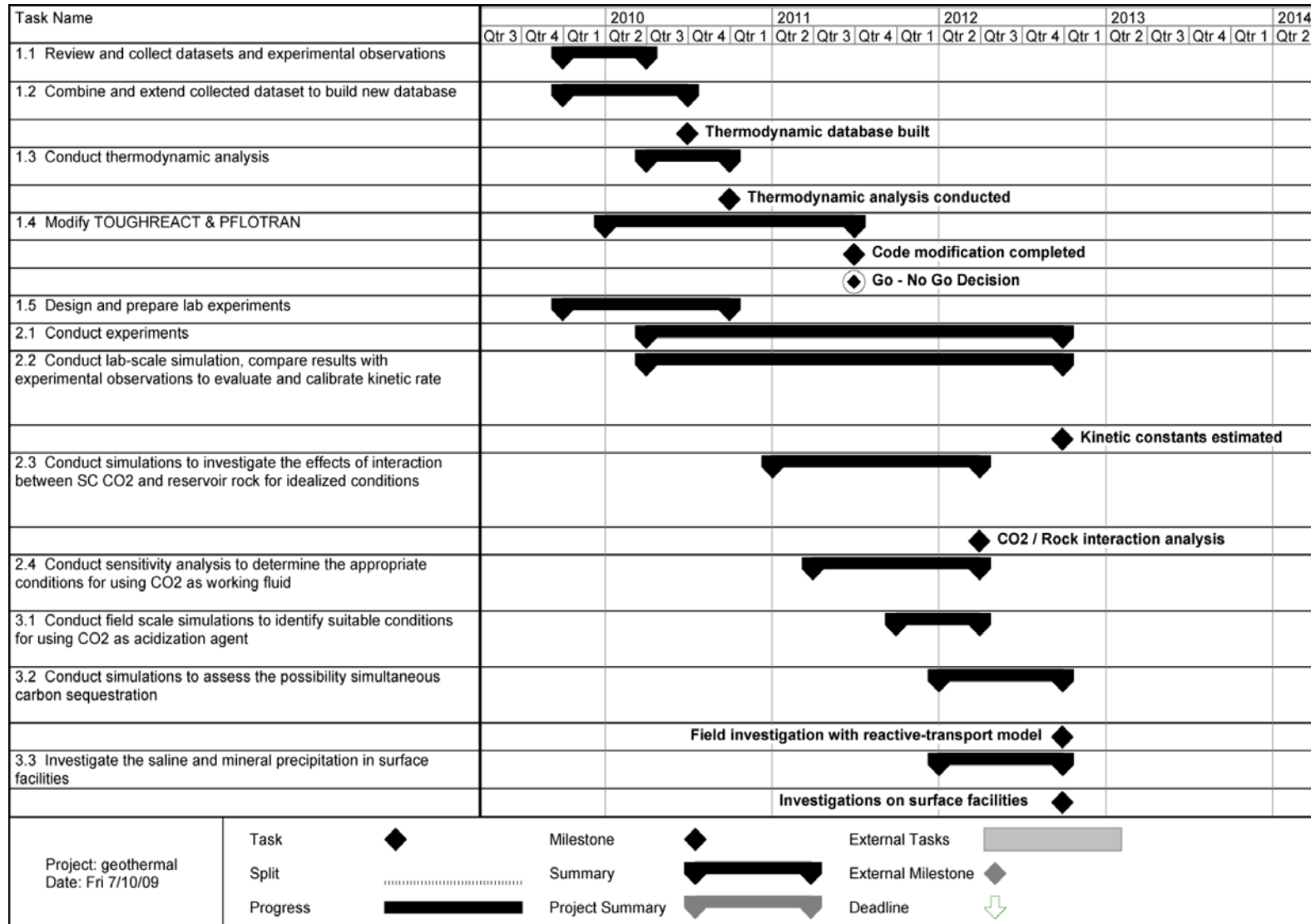
(by Dr. Lu Dr. Han, Dr McPherson, Dr. Moore and Dr. Rose at UU, Dr. Lichtner at LANL, Dr. Larson at AltaRock

Numerical simulation will take advantage of supercomputer jaguar.ccs.ornl.gov with 11,508 dual-core processors, supported by DOE SciDAC II program)

- ## Summary

- The work will be conducted over a three-year period under a single contract to the University of Utah.
- The Principal Investigator will be responsible for the overall management of the project and coordination of the tasks among the researchers.
- By working cooperatively with industry personnel, we will insure that they are kept aware of our progress and results. These results will be clearly documented and scientifically defensible.
- Quarterly and yearly reports prepared by the researchers will be compiled and submitted to the Program Administrator by the Principal Investigator.

Schedule



- Improve thermodynamic databases to include wider temperature and pressure ranges than those currently available in existing simulators for application to geothermal reservoirs [M1] (FY10)
- Determine applicable chemical reactions between water, rock, and CO₂ through thermodynamic analyses[M2]; estimate respective kinetic rates of chemical reactions [M4] (FY10,11,12)
- Develop reactive-transport model by modifying existing simulator [M3] (FY 11)
- Evaluate water/brine displacement by CO₂, water recharge, geochemical reaction processes and effects on EGS reservoirs by lab- and field-scale numerical simulations [M5]
- Assess CO₂ leakage risk and the possibility of concurrent geothermal energy extraction and carbon sequestration [M6]
- Investigate the possibility of using CO₂ as an acidization agent in EGS reservoirs [M6]
- Investigate mineral precipitation in EGS surface facilities [M7]

Go/No-Go redirections

- the new database and thermodynamic analyses cannot be completed because of lack of critical data necessary for performing EGS simulations;

We may still be able to continue with the project by adapting certain estimates and hypotheses, and our experimental program will be redesigned to test and refine these estimates and hypotheses, depending on the significance to EGS operation.

- An explicit fracture model or the dual continuum model combined with chemical reactions is computationally too demanding to carry out practical calculations for an EGS.

We can reduce the complexity of the system by limiting the number of fractures, minerals and aqueous species, etc. to make the simulations feasible, though the applicability of these results to real EGS system may be compromised to some extent.

The scope of the project addresses “Supercritical Carbon Dioxide/Reservoir Rock Chemical Interactions”, by developing a chemical and kinetic model that predicts mineral precipitation and dissolution within the EGS reservoir and in EGS surface facilities.

- Databases will be assembled and/or updated to include thermodynamic and kinetic rates for water/brine/rock/CO₂ interactions over a range of P-T conditions.
- Laboratory experimental work will be conducted to verify the database results.
- A reactive-transport model will be developed by modifying existing open source subsurface reactive flow and transport simulators (TOUGHREACT and PFLOTRAN).
- Simulations using the modified codes will be conducted to investigate the interactions between injected SC CO₂ and EGS reservoir fluids and rocks.
- The possibilities and suitable conditions of using CO₂ as a working fluid, as an acidization agent, and the simultaneous operation of CO₂ geologic storage (sequestration) and geothermal heat extraction will be explored by numerical simulation.
- Simplified numerical simulations will investigate mineral and salt precipitation in production wells and surface equipment.

Supplemental Slides

- List any publications and presentations that have resulted from work on this project. Use at least 12 point font.

Note: This slide is for the use of the Peer Reviewers only – it is not to be presented as part of your oral or poster presentation. These Supplemental Slides will be included in the copy of your presentation that will be made available to the Reviewers.

- EGS Demonstration Projects
 - Demonstrate reservoir creation that achieves a flow rate of 20 kg/s by 2015
 - Achieve a 10% increase in flow rate for EGS field site demonstration by 2011
 - Model the reservoir conductivity at an EGS system demonstration by 2011
 - Determine actual (baseline) pre-stimulation reservoir flow rate for at least one EGS field site by 2010
- EGS R&D
 - Complete the testing of a transducer for high temperature (up to 300 Degrees Celsius) ultrasonic fracture imaging tool by 2011

This slide is for reference only and is not to be included in the presentation

- Validation of Innovative Exploration Technologies
 - Confirm 400 MW of geothermal energy capacity
 - Validate two new exploration methods
- Low Temperature Demonstration Projects
 - Demonstrate the development of at least 20 MW using low temperature, co-production with oil and gas and/or geopressured resources
- Ground Source Heat Pumps
 - Reduce levelized cost of electricity (\$/ton) by 30% by 2016

This slide is for reference only and is not to be included in the presentation