FINAL REPORT

Development of coupled reactive fluid flow models

Project ID:	09-01-003
Coordinator:	Hannes Jónsson, University of Iceland
Start date:	April 1. 2009
Duration:	3+ years
Partners:	Reykjavík Energy and Lawrence Berkeley Labs

1 Project summary

The project involved the development of a coupled reactive fluid flow model including various reactions of water phase with basalt so as to mimic Icelandic geochemistry within the TOUGH-REACT software and the development of a new method, GOUST, for fitting model parameters using the iTOUGH inverse modeling software. These tools were applied in studies of CO_2 sequestration at Hellisheidi, as well as a model of the Laugarnes low temperature geothermal area. The results of this work have been described in four publications in ISI journals and two extended conference abstracts, in addition to numerous (more than 10) oral presentations and poster presentations at conferences and workshops. Only a very brief summary of the results will be sketched here, the interested reader is directed to the published articles, see section 4.

A large scale simulation of the sequestration of CO_2 in the Hellisheidi area was carried out using the TOUGH-REACT software. The results are published in [1]. In preparation for this, an extensive thermodynamic and kinetic database of the relevant chemical reactions had to be constructed and tested, as described in [2], and a detailed study of the dissolution rate of basalt carried out, as described in [3]. This extensive work was the Ph.D. research project of Edda S. P. Aradóttir and it was carried out in collaboration with Eric Sonnenfeld at Lawrence Berkeley Labs in California (an expert in TOUGH-REACT), Grímur Björnsson (an expert in geothermal modeling) and Berg Sigfússon (who carried out experiments on basalt dissolution). A key finding of this modeling work was the need for elevated temperature in order for carbonates to form and the quantitative estimation of the extent to which CO_2 will be captured by mineralization. The reactive transport simulations of the pilot injection predicted 100% CO_2 mineral capture within 10 years and cumulative fixation per unit surface area of 5000 tonnes/km^2. Corresponding values for the full-scale scenario were 80% CO_2 mineral capture after 100 years and cumulative fixation of 35,000 tonnes/km2. The CO_2 sequestration rate is predicted to range between 1200 and 22,000 tonnes/year in both scenarios. These simulations have served as a guide to the pilot study at Hellisheidi which was started subsequently. The interested reader is referred to [1] for a detailed description of the simulations and the results.

The goal was then to model a low temperature geothermal area where data had been collected over an extended period of time. The Laugarnes area in Reykjavík was selected for this purpose. As a preliminary project, an efficient procedure for parametrizing models with multiple parameters was undertaken by coupling a global optimization method with the iTOUGH software. The problem addressed here is the fact that objective functions describing how well model prediction agree with experimental observations can have multiple minima and the task of determining optimal values for the model parameters can, therefore, challenging. The goal is both to find the global minimum of the objective function rather than just some local minimum as well as an assessment of the uniqueness of the optimal parameter set. A model was developed for the Laugarnes geothermal area and the problem of multiple local minima of the objective function illustrated along with a new, global optimization method called GOUST. This work is described in [4]. Preliminary stages of this work based on long time scale annealing simulations and the AKMC method were presented earlier in two conference proceedings, see [5,6]. This work is part of Manuel Plasencia's Ph.D. project, but

the funding from GEORG was depleted before he could proceed with the model of the Laugarnes area. He is currently completing his Ph.D. thesis project by developing further the GOUST method with funding from another project (funded by the Icelandic Research Fund). Manuel is scheduled to defend his thesis early next year.

2 Project Management

The project was managed by Prof. Hannes Jónsson at the University of Iceland. The financial administration and bookkeeping was done by the budget office of the Science Institute of the University of Iceland, managing director Sigurður Guðnason (sgudna@hi.is).

3 Student involvement

Two Ph.D. students at the University of Iceland were funded by the project:

1. Edda S. P. Aradóttir, already graduated and is now employed by Orkuveita Reykjavikur.
2. Manuel Plasencia, scheduled to graduate in February 2014.

Edda S. P. Aradóttir worked on the development of the database, implementation of the Icelandic geochemical reactions in teh TOUGH-REACT code and simulation of CO_2 sequestration in the Hellisheidi geothermal field. Manuel Plasencia worked on the development of the model of the Laugarnes area and the development of a new mehod, GOUST, for determining model parameters from observations based on inverse modelling with the iTOUGH software.

Both students have given numerous presentations of this work at conferences. Most notably, Manuel won a prize for his Ph.D. student presentation at the 4th European Geothermal Ph.D. Day in Hungary in May 2013.

4 Publications and disseminations

1. 'Multidimensional reactive transport modeling of CO2 mineral sequestration in basalts at the Hellisheidi geothermal field, Iceland', E.S.P. Aradóttir, E.L. Sonnenthal, G. Björnsson and H. Jónsson, Int. J. Greenhouse Gas Control 9, 24 (2012). Available at http://www.sciencedirect.com/science/journal/17505836/9
2. 'Development and evaluation of a thermodynamic dataset for phases of interest in CO_2 mineral sequestration in basaltic rocks', E.S.P. Aradóttir, E.L. Sonnenthal and H. Jónsson, Chemical Geology 304-305, 26 (2012). Available at http://www.sciencedirect.com/science/journal/00092541/304-305
3. 'Dynamics of basaltic glass dissolution – Capturing microscopic effects in continuum scale models', E.S.P. Aradóttir, B. Sigfússon, E.L. Sonnenthal, G. Björnsson and H. Jónsson, Geochimica et Cosmochimica Acta 121, 311 (2013). Available at http://www.sciencedirect.com/science/journal/00167037/121

4. 'Global Optimization of Reservoir Models by Mapping Out Object Function Minima and Saddle Points', M. Plasencia, A. Pedersen, A. Arnaldsson and H. Jónsson, Proceedings of the Thirty-Seventh Workshop on Geothermal Reservoir Engineering at Stanford University, Jan. 30 - Feb. 1 (2012). Available at https://notendur.hi.is//~hj/papers/paperInvGeoThRes12.pdf

5. 'Geothermal model calibration using a global minimization algorithm based on finding saddle points as well as minima of the objective function', M. Plasencia, A. Pedersen, A. Arnaldsson and H. Jónsson, Proceedings of THOUGH Symposium 2012, Lawrence Berkeley National Laboratory, Sept. (2012). Available at https://notendur.hi.is//~hj/papers/paperTOUGHsymp12.pdf

6. 'Geothermal model calibration using a global minimization algorithm based on finding saddle points as well as minima of the objective function', M. Plasencia, A. Pedersen, A. Arnaldsson, J-C. Berthet and H. Jónsson, Computers and Geosciences (in press, doi: 10.1016/j.cageo.2013.09.007). Available at http://www.sciencedirect.com/science/article/pii/S0098300413002471

5 Cost statement

The funds were used to pay the two Ph.D. students, Edda S. Aradóttir and Manuel Plasencia research assistant salary. The schedule of payments was as follows:

Year 1., April 2009 - March 2010:

Salary of Edda og Manuel , 1220 kkr. Other financial support was provided by the Doctoral Student fellowship fund of the University of Iceland and the Science Institute of the University of Iceland.

Year 2., April 2010 - March 2011:

Salary of Manuel, 12 x 280 kkr = 3360 kkr

Year 3., April 2011 - March 2012:

Salary of Manuel, 7 x 297 kkr = 2080. The rest of his salary was provided by a grant from the Icelandic Research Fund.

The students attended several conferences and presented their work. The cost of these trips was covered by contributions from various other resources including the University of Iceland Graduate Student Travel Fund and The Science Institute of the University of Iceland.

The computer simulations were mainly carried out on the computer cluster Sol which was purchased with funds from the Icelandic Research Instrument Fund with matching funds provided by the University of Iceland.

The TOUGH-REACT and iTOUGH software was made available by Lawrence Berkeley Laboratories in California, USA.