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Title of Ph.D. thesis: Computational study of chemical changes in Icelandic geothermal areas: Coupling chemical reactions into reservoir models.

Description:
Reservoir models have, in the recent years, become important tools in the development of sustainable geothermal utilization. It is therefore important that they contain accurate information about the areas in question. Coupling chemical reactions into regular geothermal reservoir models is thus of great significance.

TOUGHREACT is a numerical simulation program that can be used to model chemically reactive non-isothermal flows of multiphase fluids in porous and fractured media. The code was developed at Lawrence Berkeley National Laboratory (LBNL) in California. In this Ph.D. project, TOUGHREACT will be used to simulate chemical changes in Icelandic geothermal areas with a special focus on fixation of CO2 of geothermal origin into relatively fresh basaltic lavas. The project also includes adaption of TOUGHREACT to Icelandic environment as various thermodynamic and kinetic parameters, developed in Iceland, will be introduced to the code. Models resulting from this work will be unique in Iceland as they couple chemical reactions into ordinary Icelandic geothermal reservoir models.

Reykjavík Energy, the Institute of Earth Sciences at the University of Iceland and the Earth Sciences Division at Lawrence Berkeley National Laboratory are collaborators to the project.

Supervisors: Dr. Hannes Jónsson, Department of Chemistry, University of Iceland and Dr. Grímur Björnsson, Reykjavik Energy and Reykjavik Energy Invest.

Education: M.Sc. in Theoretical Physical Chemistry from the University of Iceland, 2006 and B.Sc. in Chemical Engineering from the University of Iceland, 2004

Papers and abstracts:

- **E.S. Aradóttir** and H. Jónsson, in preparation (2007).*Trends in structure and stability of magnesium-3d transition metal hydrides*.
- **E.S.P. Aradóttir**, L.G. Camargo, H. Jónsson, N. Kitamura, D. Kyoi, D. Moser, T. Sakai, T. Taniguci and H. Yusa, in preparation (2007). *Metastable magnesium transition metal hydrides with large hydrogen storage capacity and fast hydrogen diffusion*.
- **E.S. Aradóttir,** 2006. *Theoretical calculations on magnesium transition metal hydrides: structure, stability and diffusivity.* M.Sc. thesis, University of Iceland.
- **E.S. Aradóttir,** 2005. *Compilation and interpretation of chemical monitoring data from low-temperature geothermal fields in the Reykjavík area*. Report no. 22-2005, Reykjavik Energy.
- **E.S. Aradóttir**, 2004. *Production history and reservoir parameters for some low-temperature fields in SW-Iceland.* Report no. 19-2004, Reykjavik Energy.

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