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To: LES (Laboratory for Waste Management)

Cc: SN, CL, BL, TD, AL

Villigen PSI, 08 July 2016

Extraordinary LES Palaver

Time and Place: Friday 22.07.2016, 10:00-11:30, OFLA/209

Title: Application of the MINES thermodynamic database to simulate crustal fluid-rock systems

Speaker: Prof. Alexander P. Gysi, Colorado School of Mines, Golden CO, USA (agysi@mines.edu)

Summary:

Professor A. Gysi's research group is involved in the development and testing of internally consistent thermodynamic data for modeling ore forming processes using GEM-Selektor with the recent launch of the MINES thermodynamic database (http://tdb.mines.edu). A major problem for modeling fluid-rock reactions in different geologic systems is the selection of adequate activity models and the availability of thermodynamic data for aqueous species, gases and minerals. Two different research projects will be presented, in which the group applies the MINES database to various geoscientific problems. The first project stems from the past collaborations in the Carbfix project in Iceland applied to the prediction of CO_2 sequestration into basaltic rock formations. The CO_2-water-basaltic glass batch type experiments were combined with numerical simulations to determine changes in the resulting mineralogy and fluid chemistry as a function of time, temperature (40 to 200 °C), acid supply (pCO_2 to 20 bar), and fluid/rock ratios. The second project relates to research from the crustal fluid-rock interaction lab at Colorado School of Mines and is applied to the behavior of REE in hydrothermal fluids relevant to the formation of REE mineral deposit. The lack of consistent thermodynamic data for REE-bearing mineral solid solutions led to start a series of solubility and calorimetric studies on REE fluorocarbonates and phosphates, and hydrothermal REE-fluid-calcite partitioning experiments. The overall goal of the MINES database is to stimulate an open access critical evaluation of thermodynamic data among a network of researchers.

Everybody who has an interest is welcome!
Dmitrii Kulik