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Reactive transport simulation by combining a multiphase-capable transport code for unstructured meshes with Gibbs energy minimization and multi-electrolyte solution models

Sarah Jane Fowler (1), Ferdinand Hingerl (2), Thomas Driesner (1), Georg Kosakowski (2), Dmitrii Kulik (2), and Thomas Wagner (1)

(1) Institute of Geochemistry & Petrology, ETH Zurich, Zurich, Switzerland (sarah.fowler@erdw.ethz.ch), (2) Laboratory for Waste Management, Paul Scherrer Institut, Villigen PSI, Switzerland (ferdinand.hingerl@erdw.ethz.ch)

We present a novel C++-based computational tool for modelling temporally and spatially varying chemical interactions between hydrothermal fluids and rocks that may affect the long-term performance of geothermal reservoirs. It incorporates fluid–rock interaction and scale formation self-consistently, via a modular coupling approach that combines the Complex System Modelling Platform (CSMP++) code for fluid flow in porous and fractured media (Matthai et al., 2007) with the numerical kernel (GEMIPM2K) of the GEM-Selektor (GEMS) Gibbs free energy minimization package (Kulik, Wagner et al., 2007). CSMP++ uses finite element–finite volume spatial discretization, implicit or explicit time discretization, and an operator splitting approach to solve equations. GEMS supports a variety of equation of state and activity models, facilitating calculation of complex fluid-mineral equilibria.

We previously modified GEMS for improved application to geothermal conditions via implementation of the standard Pitzer (Harvie et al., 1984) and alternative EUNIQUAC (Thomsen et al., 1996) models. Here we present the ELVIS multi-electrolyte solution model. ELVIS is based on reformulation and re-parameterization of the existing EUNIQUAC model to address several conceptual and technical deficiencies. ELVIS is well-suited to saline solutions at increased P and T.

A critical advantage of the coupled code compared to existing hydrothermal reactive transport models is simultaneous consideration of complex solid solutions (e.g., clay minerals) and non-ideal aqueous solutions.

Each coupled simulation results in a thermodynamically-based description of the geochemical and physical state of a hydrothermal system evolving along a complex P-T-X path. The code design allows efficient, flexible incorporation of numerical and thermodynamic database improvements.

We verify the coupling scheme via comparison of results to a well-known calcite–dolomite system benchmark (Engesgaard & Kipp, 1992; Prommer, 2002; Shao et al., 2009). We apply the coupled code to selected geologic applications, including a granitic system and a faulted geometry, to test its accuracy and performance.

Engesgaard, P. & Kipp, K. L. (1992). A geochemical transport model for redox-controlled movement of mineral fronts in groundwater flow systems: a case of nitrate removal by oxidation of pyrite. Water Resources Research 28, 2829–2843.

Harvie, C. E.; Møller, N. & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: the Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25°C. Geochimica et Cosmochimica Acta 48, 723–751.

Kulik, D., Wagner, T. et al. (2007). GEM-Selektor (GEMS-PSI) home page, Paul Scherrer Institut. Available at http://gems.web.psi.ch. Accessed 2 September, 2010.

Matthäi, S. K., Geiger, S., Roberts, S. G., Paluszny, A., Belayneh, M., Burri, A., Mezentsev, A., Lu, H., Coumou, D., Driesner, T. & Heinrich C. A. (2007). Numerical simulation of multi-phase fluid flow in structurally complex reservoirs. In: Jolley, S. J., Barr, D., Walsh, J. J. & Knipe, R. J. (eds.) Structurally Complex Reservoirs. Geological Society, London, Special Publications 292, 405–429.

Prommer, H. (2002). A Reactive Multicomponent Transport Model for Saturated Porous Media, User's Manual Version 1.0. Contaminated Land Assessment and Remediation Research Centre. The University of Edinburgh, UK.

Shao, H., Dmytrieva, S. V., Kolditz, O., Kulik, D., Pfingsten, W. & Kosakowski, G. (2009). Modeling reactive transport in non-ideal aqueous–solid solution system. Applied Geochemistry 24, 1287–1300.

Thomsen, K. Rasmussen, P. & Gani, R. (1996). Correlation and prediction of thermal properties and phase behaviour for a class of aqueous electrolyte systems. Chemical Engineering Science 51, 3675–3683.