Embedding 'Rich Chemistry' into Reactive Transport Modeling of Hydrothermal Systems

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Chemically plausible systems of relevance in geothermics and ore geochemistry may involve aqueous electrolyte, non-ideal mixed fluids, melts and solid solutions, redox transitions, sorption, and kinetic entrapment of elements. This complexity is captured in 'rich-chemistry' thermodynamic models valid for wide *P* & *T* ranges, based upon internally consistent databases of thermodynamic properties [1,2], models of mixing [3], and kinetic rates, and solved using advanced methods of Gibbs energy minimization (GEM).

In geomedia, reactive transport (RT) phenomena occur where heterogeneous chemical reactions are driven by the advective or diffusive transport of aqueous or gaseous fluids. Mineral growth or dissolution may lead to modifications of the pore space and changes of transport properties with time. To simulate the medium evolution, such feedbacks require coupling the non-isothermal transport model to a solver of partial chemical equilibria at each control volume and time.

For embedding the 'rich chemistry' into RT simulations, GEM codes in GEMS3K [4] and in Reaktoro [5] appear to be superior to popular LMA (law of mass action) codes such as MINEQL or PHREEQC. The main reason is that GEM uses the complete thermodynamic information for all chemical substances in all phases included into the system, whereas LMA methods neglect the stability values for the 'master' species, thus utilizing much less input thermodynamic data.

Regarding hydrothermal systems, two main areas of RT modeling are geothermal resevoirs [6] (optionally with CO_2 disposal [2]) and ore formation processes [7]. They have a lot in common, although some RT phenomena (e.g. localized deposition of secondary minerals) beneficial for ore formation may be harmful for geothermal systems (clogged fractures, mineral scales in pipes). Recent RT simulations with the new CSMP++GEM coupled code [8,9], also related to the Sinergia COTHERM2 project, will be discussed in this context.

[1] Miron et al. (2016) *GCA* **187**, 41-78. [2] Gysi (2017) *PAC,* in press. [3] Wagner *et al*. (2012) *Can. Miner*. **50**, 1173-1195. [4] Kulik *et al*. (2013) *Computat. Geosci*. **17**, 1-24. [5] Leal *et al*. (2016) *AWR* **88**, 231-240. [6] Scott *et al*. (2015), *Nat. Comm*. **6**, 7837. [7] Weis et al. (2012) *Science* **338**, 1613-1616. [8] Yapparova *et al*. (2017) *TiPM*, online. [9] Yapparova *et al*. (2017) *MinMag*, this volume.