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THERMODYNAMICS OF AQUEOUS SOLUTIONS AT HIGH IONIC STRENGTH USING THE PITZER MODEL

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More and more attention is paid to the description of brine chemistry for various reasons. Natural brines are extensively exploited for the reserves of valuable chemical elements or chemical products they contain (such as lithium, potash, potassium, magnesium and other various salts). Geothermal energy currently uses hot deep brines. Greenhouse gases like CO_2 are forecasted to be stored in deep geological reservoirs containing saline solutions. The number of desalination plants is increasing with the fresh water demand, leading to increasing amounts of highly saline waste.
Geochemical modelling is one of the numerical tool needed to predict the properties and the behavior of such systems. Different approaches can be used but one of the most relevant is the Pitzer[1] model.
Since more than 20 years, our team is working on developing and improving the modelling of multicomponent saline systems, using the Pitzer approach. Our efforts focus on both the development of a database for specific interaction parameters and a numerical code. We propose a Pitzer database for several chemical systems in order to deal with lithium chemistry[2,3], phosphate systems, chloride systems (Na^+, K^+, Ca^{+2} and Mg^{+2})-Cl between 0-100°C[4], and nitrate-sulfate systems[5] at 25°C, both in acidic and basic conditions. These implementations in the database allow dealing with topics such as the optimisation of lithium extraction process from salars brines or the improvement of phosphate production from WPPA process. Next evolution perspectives of this database are the extension to high temperatures (above 150°C) and the addition of trace elements (aluminium and radionuclides for instance).
The description of these complex aqueous solutions requires the development of specific tools, like PhreeSCALE[6], after the geochemical code PHREEQC[7]. In this new tool, computation of heat capacities, excess enthalpy and density was implemented in coherence with Pitzer and HKF[8] models. Consequently, the heat capacity or density of a geothermal fluid can be computed according to its exact chemical composition.

References:

(1) Pitzer, K. S. **1991** *Activity Coefficients in Electrolyte Solutions*
(2) Lassin, A.; et al. *Am. J. Sci.* **2015**, *315*, 204–256 10.2475/03.2015.02.
(3) Lassin, A.; et al. *CALPHAD accepted*.
(4) Lach, A.; et al. *J. Chem. Eng. Data* **2017**, *62* (10), 3561–3576 10.1021/acs.jced.7b00553.
(5) Lach, A.; et al. *J. Chem. Eng. Data* **2018**, *in press* 10.1021/acs.jced.7b00953.
(6) Lach, A.; et al. *Comput. Geosci.* **2016**, *92*, 58–69 10.1016/j.cageo.2016.03.016.
(7) Parkhurst, D. L.; Appelo, C. A. J. **2013** *Description of Input and Examples for PHREEQC Version 3*
(8) Helgeson, H. C.; et al. *Am. J. Sci.* **1981**, *281*, 1249–1516 10.2475/ajs.281.10.1249.