Improvements in Pitzer's database for calculating CO_2 solubility in the Na-Ca-Cl saline aqueous systems

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Methodology

Original experimental data from the NaCl-CO_2-H_2O and $CaCl_2$-CO_2-H_2O systems at high temperature, high pressure and high salt concentration are used to define new interactions parameters between CO_2 and dissolved ions for the implementation of the Pitzer database. The optimization was made using PEST[1], a computational optimization software, whereas the chemical equilibria are computed using the PhreeSCALE[2] software.

Discussions

After optimizing the interaction parameters, the numerical simulations allow describing the experimental data, thus reducing the deviations between the PhreeSCALE results and the experimental data. Interaction parameters are valid from low to high pressures (200 bars), temperatures and ionic strengths up to 423 K and 6 eq/kgw, respectively.

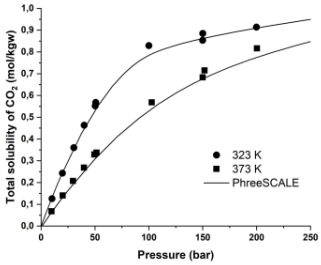

Figure 1: Experimental and calculated solubility of CO_2 in a 1 mol/kgw $CaCl_2$ solution at 323 and 373 K.

[1] Doherty J. (2004) PEST. Model-independent parameter estimation. User manual: 5th Edition.

[2] Lach et al. (2016) - Thermal and Volumetric Properties of Complex Aqueous Electrolyte Solutions Using the Pitzer Formalism – The PhreeSCALE Code. Comput. Geosci, 92, 58−69.