A simplified approach for density calculation for up to hexary brine solutions

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Density-driven flow not only plays an important role for geothermic issues or in the field of groundwater exploration in coastal areas but also for radioactive waste disposal near or in salt formations. Modelling programs commonly use methods to calculate densities of complex, high-saline salt solutions using total concentrations only, but ignoring non-ideal mixing effects. Thus, only rough approximation of the density of brines can be achieved.

To increase the accuracy of density calculations we developed a new approach (subsequently named GRS model) for future implementation in transport codes (e.g. TOUGHREACT). Our approach, based on the ionic charge, was reviewed for its conformity to experimental data and also compared with other, more sophisticated approaches: the Pitzer approach [1] and the method of Laliberté and Cooper [2]. Contrary to the Pitzer approach [1], where over 80 parameters are necessary, our method requires only 4 parameters. Binary to hexary systems of brine like the IP21 solution (saturated with polyhalite, halite, carnallite, kainite, sylvite) were considered.

We found that predictions of densities for even hexary systems of brine up to high ionic strengths (17,3 mol/kg) can be achieved. The highest mean differences to experimental data are found for quinary systems with 0.008 g/cm^3 for the GRS model and 0.003 g/cm^3 for the Pitzer approach. Thus, these results for modeled densities have an accuracy of < 0.01 g/cm^3.

[1] Krumgalz, Pogorelsky & Pitzer (1995), J. Sol. Chem. **24**, 1025-1038. [2] Laliberté & Cooper(2004), J. Chem. Eng. Data **49**, 1141-1151.