Thermodynamic database for iron in high-saline solutions

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Introduction

As major constituent of containments for the disposal of radioactive waste, iron has a considerable impact on geochemical conditions in the near-field of underground repositories. The large variety of ferrous and especially ferric species poses a challenge for the development of a chemical model, which should be easy enough to allow for the assignment of thermodynamic data, and at the same time should be detailed enough to cover solubility relations of the most relevant solid phases.

Description of the work

For ferrous and ferric iron, only one species each was assumed to be predominant under specific conditions, Fe^{2+} and $Fe(OH)_4^-$. For ferrous iron Pitzer coefficients were developed from isopiestic data. Standard thermodynamic data were adopted from [1] and [2].

Solid phases and their thermodynamic standard data were selected from [1] and [3]. Wherever possible, data were selected to be consistent with the NEA-database [1] unless solubility data suggested otherwise.

Activity coefficients for aqueous solutes were calculated applying the Pitzer formalism [4]

Results

Considering undersaturated aqueous solutions, ferrous activities can be reproduced well for a number of systems. Solubility modeling of solid ferric phases indicate the necessity to consider one more ferric species for pH<6. This is subject of ongoing work.

[1] Lemire (Chairman) (2013) Vol 13a: Chemical Thermodynamics of iron. Part 1, OECD Nuclear Energy Agency Data Bank, Eds., OECD Publications, Paris, France, (2013). [2] Diakonov et al. (1999) *Geochim. Cosmochim. Acta*, **63**, 2247–2261. [3] Hagemann et al., Project report, 02 C 1244. GRS-260, ISBN 978-3-939355-35-9. [4] Pitzer (1973) J. Phys. Chem. **77**, 268.