
A comparison between aqueous solution and surface complexation models

Johannes Lützenkirchen

Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology, Germany

e-mail: johannes.luetzenkirchen@kit.edu

A comparison between complexation models in aqueous solutions and on mineral surfaces is given. Various aspects are addressed including the treatment of activity coefficients and multi-dentate complexes, the role of ion-pairs, or the relation between hydrolysis of cations in solution and at interfaces.

The surface potential vs. pH relationships at a given salt level are the most important property related to non-ideality in modelling surface complexation equilibria. They are discussed in numerous disciplines in terms of model results and more recently also in terms of experimental results as related to more easily accessible measurements of zeta-potential [1]. The precise dependence on salt level is under debate. In solutions the variation of the activity coefficient is typically strongly affected when the electrolyte concentration is varied up to saturated salt solutions, while the pH-dependence is negligible.

This and the intervening role of ion-pairs [2] is discussed in some detail based on published parameter sets with focus on the differences between solution and surface reactions.

References

- [1] T. Preocanin *et al.*, *Environmental Chemistry* **14**, 295-309 (2017).
- [2] J. Lützenkirchen, *Journal of Colloid and Interface Science* **195**, 149-155 (1997).