

Comparison of model and experimental results for CO₂-water-rock interactions: what data are best?

HENTSCHER, M.^{1*}, OSTERTAG-HENNING, C.¹,
STADLER, S.¹ AND WALDMANN, S.¹

¹Bundesanstalt für Geowissenschaften und Rohstoffe,
Stilleweg 2, D-30655 Hannover, Germany
(*correspondence: Michael.Hentscher@bgr.de)

Thermodynamic modeling is a common tool to understand water-rock interaction processes. Inverse modeling is commonly used for understanding alteration processes which lead to the actual fluid and/or rock composition; in contrast, a forward modeling approach can be used to predict reaction processes. In the context of CO₂ sequestration, we apply thermodynamic forward modeling to predict mineral reactions which are induced by the acidification of the aquifer.

The quality of modeling results depends on both the careful definition of boundary conditions and on the quality of thermodynamic data. The selection of relevant thermodynamic data is challenging because most available data cover only a small temperature and pressure range and have been extrapolated to the range of interest. Furthermore, thermodynamic properties for certain mineral phases (e.g. smectite) are lacking and thus need to be estimated [1]. Each thermodynamic database combines data from different sources which in comparison enhances the variety of results.

Within the four year FP7 ULTimateCO2 project (2011-2015) we used available thermodynamic data for minerals and aqueous species to undertake forward modeling of solubility experiments of clay minerals (e.g. illite). The results were compared to published experimental data from the GaMin'11(e.g [2]) and COORAL projects. Aluminum species are often reported to have a significant influence on mineral dissolution [e.g. 3, 4, 5]. Our first results imply that aqueous Al has only a minor influence on mineral reactions compared to other aqueous species such as K.

Furthermore, comparison between experimental results and modeling indicates that increasing aqueous Mg-concentrations over time are controlled by ion exchange reactions rather than mineral (Mg-illite) dissolution.

[1] Wolery and Jove-Colon (2007) *YMP Technical Report*. [2] Black & Haese (2012) CO2CRC Report No: RPT12-3839. [3] Shock *et al* (1997) *GCA* **61**, 907-950. [4] Tagirov & Schott (2001) *GCA* **65**, 3965-3992. [5] Blanc *et al* (2012) *Applied Geochemistry* **27**, 2107-2116