Smart K_d-values as realistic distribution coefficients

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One important natural process retarding the transport of contaminants is sorption onto mineral surfaces. A respective process understanding and realistic geochemical modelling of sorption is thus of high relevance in safety assessments of radioactive waste repositories. Further application areas are groundwater protection, environmental remediation or e.g. disposal of chemotoxic hazardous waste. Most often conventional concepts with constant distribution coefficients (K_d-values) are applied in reactive transport simulations, with the advantage to be simple and computationally fast, but not reflecting changes in geochemical conditions.

Here, the smart K_d-concept (www.smartkd-concept.de), a mechanistic approach mainly based on surface complexation models, is applied in geochemical modelling and has been further developed to calculate more realistic distribution coefficients for a wide range of important environmental parameters, e.g. pH, ionic strenght, competing cations and complexing ligands [1, 2] using PHREEQC, UCODE and RepoSUN/SimLab [3, 4, 5]. The philosophy behind this approach is to compute a-priori multidimensional smart K_d-matrices which are available for subsequent transport simulations.

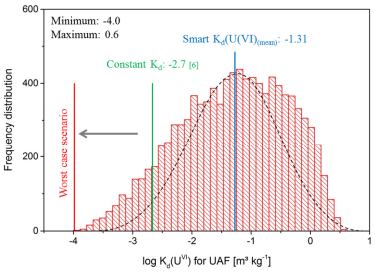

Fig. 1. Histogram of 10,000 pre-calculated log K_d-values for U(VI) (K_d in $m^3\ kg^{-1}$, logarithmic).

We could demonstrate that constant K_d-values (e.g. for U(VI) [6], see Fig. 1) used so far are too crude an assumption but they rather range over several orders of magnitude.

For considering worst-case scenarios much smaller K_d-values have to be use than in conventional concepts. Similar results will be presented for Am and Np.

[1] Noseck et al. (2012) *GRS-Report 297,* [2] Fein (2004) *GRS-Report 192*, [3] Parkhurst & Appelo (2013) *USGS Report 6-A43.* [4] Poeter et al. (2014) *GWMI 2014-02*. [5] Becker (2016) *GRS-Report 411*.