Reactive transport modeling : Application of the «smart K_d-concept»

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Objectives
- Developing better understanding of retardation processes for actinides under varying geochemical conditions in long-term safety assessments of radioactive waste repositories
- First proof of concept of the smart K_d-concept
  - Application of Eu(III) surface complexation parameters (SCPs) in reactive transport models (PhreeqC¹¹)
  - Eu(III) migration through quartz sand columns
- Comparison of surface complexation formalism as applied to batch and column experiments

Approach
- Evaluation of protolysis constants (pK-values) from surface charge (batch titration) data
- Evaluation of log K-values for Eu(III) SCPs (logK-values) from batch sorption data
- Reactive transport modeling of Eu(III) migration through quartz sand columns
  - Determination of transport parameters via STANMOD²
- Application of batch SCPs to predict Eu(III) migration under varying geochemical conditions

Results
- Application of diffuse double layer model (DDL) to determine quartz protolysis constants from titration literature data³
  - DDL pK -8.0 ± 0.1 SOH -> SO⁻ + H⁺
  - Stern model⁴ pK -7.5 SOH -> SO⁻ + H⁺
  - logKNa -9.4 SO⁻ + Na⁺ -> SONa
- Quartz mineral properties
  - Specific surface area (SSABET) 0.08 m² g⁻¹
  - Surface site density⁴ (SSD) 4.6 sites nm⁻²

Future perspectives
- Further proof-of-concept of the smart K_d-approach via
  - Evaluation of batch SCPs for orthoclase Eu(III) and muscovite Eu(III) from batch and titration experiments
  - Application of batch SCPs to reactive transport of Eu(III) through muscovite and orthoclase columns
  - Application of the smart K_d-concept to simulate Eu(III) transport through a synthetic and natural sediment
  - Continuous improvement of developed surface complexation models via state of the art spectroscopic Eu(III) surface complexation and speciation data
  - e.g. evaluation of Eu-sulfate solution and surface speciation

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