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Quantifying conservatism of performance assessment calculations by sorption model reduction : Case study on near field Cs migration in Callovo-Oxfordian clay

Eef Weetjens (1), Evelien Martens (1,2), and Diederik Jacques (1)

(1) Institute Environment, Health and Safety, Belgian Nuclear Research Centre SCK•CEN, B-2400 Mol, Belgium, eweetjen@sckcen.be, (2) Now at CSIRO.

In classical performance assessment (PA) calculations, the complex geochemical transport behaviour of some radionuclides in the near field of a geological repository is usually simplified in view of the extreme timescales that need to be computed. At a smale scale, geochemical tools, such as PHREEQC, can be used for diffusive transport calculations accounting for the complex geochemical processes. However, they are tradionally not used for diffusive transport calculations for the considered time- and spatial scales in PA. The objectives of this paper are twofold. As a starting point, the implementation of diffusive transport in a 2D radial geometry is tested by verification with another code, in casu COMSOL Multiphysics. Secondly, it is assessed whether using more complex and more realistic sorption models provide added value for a PA analysis. The latter is done by comparing results obtained with complex models considering competitive sorption processes of radionuclides and simplified models such as a linear Kd approach and a Langmuir isotherm. The case study discussed in this paper focuses specifically on migration of 135Cs from vitrified high-level waste canisters within the near field of a geological repository in Callovo-Oxfordian clay for a timeframe of a couple of thousand years. Results of the verification calculations for radial diffusive transport of a conservative tracer and a (linearly) sorbed element show an excellent agreement between concentration profiles obtained with the PHREEQC and COMSOL codes. Further application of PHREEQC using sorption models of different complexity suggests that "upscaling" of thermodynamic models to repository scale could indeed support the PA analysis. Primarily, it provides additional information on how to choose adequate (i.e. conservative) parameter values for the expected concentration range around the repository. Furthermore, comparison of results obtained with a Kd model and more complex models demonstrates quantitatively the safety margin implicitly introduced into the PA calculations through model abstraction.