

Long-Term Performance Assessment of Nuclear Waste Glasses in a Geological Repository: a reactive diffusion model called “MOS”

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Long-term performance assessment of nuclear waste glasses in a geological repository relies on multiscale modeling, from atom scale models (Monte Carlo, Molecular Dynamics) up to geochemical models and reactive transport codes. The simpler the model is, the more it requires hypotheses whose demonstrations come from smaller scales models. MOS model is an easy-to-use tool meant to assess the efficiency of the environment, as a diffusion barrier, on glass package life time. It is used to sort out the effect of key glass and environment parameters before using geochemical models and reactive transport codes.

One of the hypotheses made in MOS model is to consider silicon reactive diffusion in the environment as the main driving force for glass alteration in a water saturated media. Parameters are relative to the glass (dissolution rates, solubility, size of the glass package...) and to the environment (porosity, diffusion coefficient of Si, capacity to consume silica, temperature, time before water saturation...). Resolution is performed in spherical coordinates for successive zones of different size, diffusivity and reactivity. These are meant to represent containers, their corrosion products and the surrounding clay. An original resolution is proposed for reactive transport. It makes it possible to perform all the calculations on a simple spreadsheet.

One simple important conclusion driven by sensitivity analysis is the following : even highly diffusive and silicon consuming environments can represent an efficient barrier effect that prevents glass from dissolving at its highest rate.

Ongoing work is relative to (i) validation of MOS hypotheses by comparison in chosen disposal scenarios with a model taking into account the whole chemistry (case of GRAAL model [1] implemented in a reactive transport code) and (ii) sensitivity analysis of the influence of each input parameter on the glass package life time.

1. Frugier, P., et al., *Modeling glass corrosion with GRAAL. npj Materials Degradation*, 2018. 2(1): p. 35.