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Nuclear glass alteration: bridging the gap from surface reactivity description to reactive transport at the scale of the fractured block

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The long term behavior of the nuclear glass in deep geological storage conditions is a subject of prime importance for the nuclear industry and the science in general. It requires an in-depth understanding of the behavior of the glass dissolution and the amorphous layers development at the micro scale, as well as the effect of the diffusion, the thermal convection and certain parameters of modeled systems that govern the kinetics of the glass dissolution.

The glass matrix being highly fractured, as a result of stress release generated during the glass cooling, the treatment of such a medium demands the application of both the discrete modeling and the homogenized modeling approaches. This research starts with the study of the evolution of the amorphous layers by executing the reactive transport modeling (HYTEC transport code [1], [2]) in conjunction with the GRAAL geochemical model [3]. In the first step, the behavior of fractures is described explicitly. The influence of such parameters as number of fractures, their length and aperture as well as the volume of water in contact and water diffusion coefficient is observed (Figure1, Figure2) and explained with respect to the GRAAL model. It has been compared to experimental results (Chomat, 2008), close agreement has been reported.

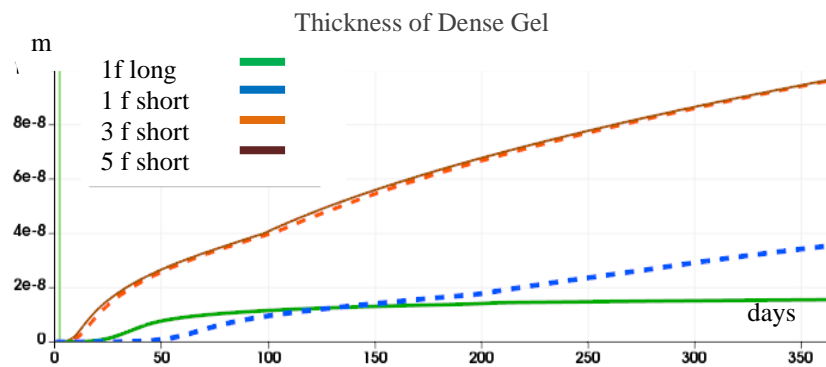


Figure1 Thickness of Dense Gel over time for different modeled objects

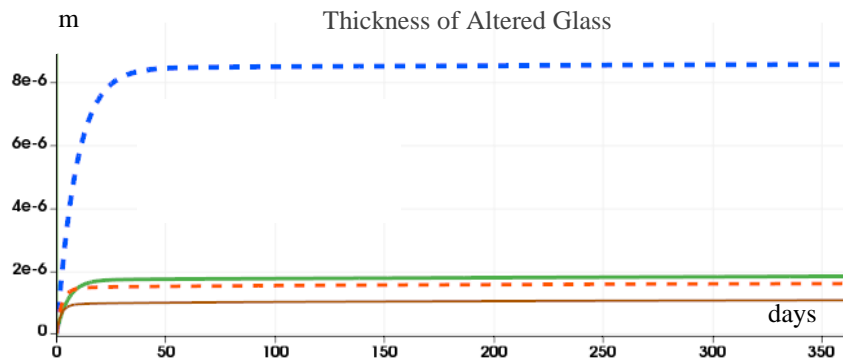


Figure2 Thickness of Altered Glass over time for different modeled object (legend of figure 1 is valid)

Following, the characterization of the fracture network by the tools of Morphological Mathematics is performed. Two entire blocks of vitrified glass are described by means of the analysis of the high quality 2D images; this thorough review includes: extraction of a fracture network and pullout zones, determination of block's crystals, calculation of fracture apertures (Figure 3) and generation of the equivalent mathematical representation of these blocks where relevant network characteristics are assigned to the centroids of crystals.

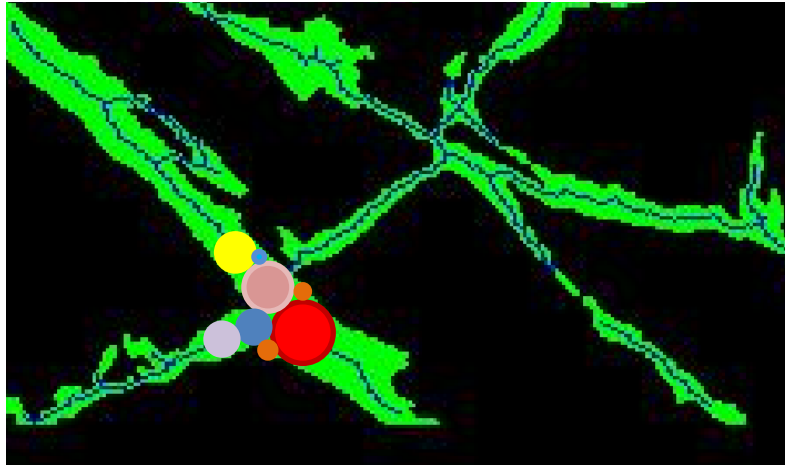


Figure3 Concept of maximal balls used to calculate fracture apertures

Next, the upscaling techniques are elaborated for flow, transport, and chemical behavior. They permit to respect the existing directional anisotropy caused by the way of glass block fabrication (two casts) and inhomogeneous release of mechanical stresses at the stage of glass solidification [4].

Furthermore, the accuracy of the proposed homogenized model is currently at the stage of verification; for instance, we are investigating whether the explicit fracture representation could be replaced by the geometrical representation by centroids of crystals and suitable tessellation (Voronoi & Johnson-Mehl); and how to adapt this geometrical representation in order not to lose the anisotropy impact on the upscaled diffusion coefficient and the coefficient of the effective equivalent permeability.

Eventually, we will carry out RTM at the scale of the fractured block, and to confirm the validity of the model, we plan to compare the results of modeling with the experimental data of the aqueous alteration of the full-scale SON68 nuclear glass block that has been altered for 7.5 years in a static reactor at LCLT laboratory.

References

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