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Modelling method for glass alteration with graal2 model

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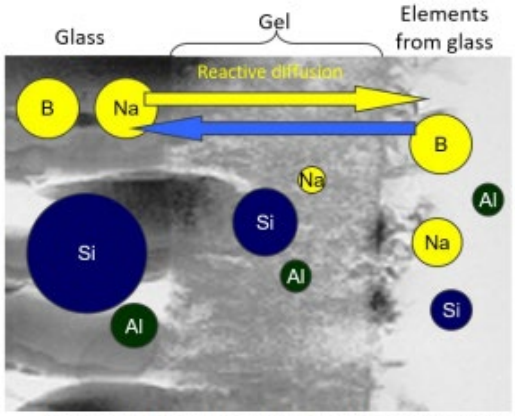

Figure 1 : Presentation of the working envirnnement

Implemented in the CHESS/HYTEC reactive transport code, the glass alteration model GRAAL 2 has been designed to analyze and forecast glass alteration experiments that occur during geological disposal in a complex chemical environment [1]. GRAAL 2 considers various phenomena like hydrolysis, interdiffusion, passivating gel formation, and potential secondary phases. Based on the GRAAL 1 model [2], this new version considers the chemical environment's impact on weathering layers and establishes a minimum density requirement for passivation.

Experiments were carried out in 2020 to analyze the alteration of a glass containing 64.9% SiO_2, - 13.6% Na_2O-17.3% B_2O_3-4.1% Al_2O_3 (Figure 1) at 90°C. The purpose of the experiments was to evaluate the capacity of the model to reproduce the phenomena observed when the chemical composition of the environment in contact with the glass changes. The main variable parameters were the altering solution's composition (sodium and silicon loaded solution) and the ratio of glass surface to solution volume.

The development of a modelling method makes it possible to determine the optimal parameters set for the modelling. The application of these parameters allows the prediction of altered glass, formed gel and precipitated secondary phase quantities. The model also gives insights into the evolution of the solution's composition over time. The findings indicate that the model can replicate the experimental results quite precisely, whether in pure water or ionic environments. This method can be included in an automatic numerical tool that enables uncertainties to be explored by increasing the available modelling outcomes. Therefore, it is possible to determine the parametric uncertainties based on experimental uncertainties and therefore to qualify the method.

[1] Frugier, P., Minet, Y., Rajmohan, N. et al (2018). Modeling glass corrosion with GRAAL. npj Mater Degrad 2, 35

[2] Frugier, P., Gin, S., Minet, Y., Chave, T., Bonin, B. et al (2008). SON68 nuclear glass dissolution kinetics: Current state of knowledge and basis of the new GRAAL model. Journal of Nuclear Materials, Elsevier, 380 (1-3), pp.8-21