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# Long-term geochemical modeling with GRAAL2

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Presented at the 2023 Goldschmidt conference, the GRAAL 2 model has been incorporated into the CHESS/HYTEC reactive transport code to predict the alteration of glasses used for radioactive wastes confinement [1] under geochemical disposal conditions [2]. GRAAL 2 takes into account hydrolysis, Interdiffusion, protective gel formation, secondary phases precipitation leveraging geochemical databases and reactive transport in the environment through Hytec.

During the last Goldschmidt conference, the methodology for parametrizing the model and the result that can be obtained were presented. This was demonstrated through an application on two experiments performed on a simple glass of 4 oxides (SiO<sub>2</sub> – B<sub>2</sub>O<sub>3</sub> – Na<sub>2</sub>O – Al<sub>2</sub>O<sub>3</sub>) at 90°C in pure water [3]. An uncertainty study qualified the method and the results of the model on these experiments. It revealed that the model's prediction closely matched the experimental data. At the 2023 Migration conference, results for the same glass were presented, highlighting the ability to take into account variations in the solution composition and in the glass surface-to-volume ratio therefore confirming that the model was perfectly able to predict these kinds of effects.

This year, after a short presentation of the model, a 25-year experiment on the same simple glass is modelled to discuss the model's ability to predict long-term experimental results. Initially the parameters determined from last year's experiments are used. Some discrepancies with the experiment are discussed. Then a new set of optimized parameters is proposed to drive the discussion relative to the mechanisms at work over the course of such a long experiment.

To conclude, the model's capacity, parameterization method, and results are discussed to evaluate the overall model's performance.

[1] Zanini, R., Franceschin, G., Cattaruzza, E. *et al.* A review of glass corrosion: the unique contribution of studying ancient glass to validate glass alteration models. *npj Mater Degrad* **7**, 38 (2023). <https://doi.org/10.1038/s41529-023-00355-4>

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

[3] DELCROIX, Maxime. Modelling method for glass alteration with graal2 model. In : *Goldschmidt 2023 Conference*. GOLDSCHMIDT, 2023.