Predicting Radioactive Waste Glass Viscosity, Density and Dissolution with Machine Learning

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Abstract : The vitrification of high-level nuclear waste within borosilicate glass and its incorporation within a multi-barrier repository deep underground is widely accepted as the preferred disposal method. However, for this to happen, any safety case will require validation that the initially localized radionuclides will not be considerably released into the near/far-field. Therefore, accurate mechanistic models are necessary to predict glass dissolution, and these should be robust to a variety of incorporated waste species and leaching test conditions, particularly given substantial variations across international waste-streams. Here, machine learning is used to predict glass material properties (viscosity, density) and glass leaching model parameters from large-scale industrial data. A variety of different machine learning algorithms have been compared to assess performance. Density was predicted solely from composition, whereas viscosity additionally considered temperature. To predict suitable glass leaching model parameters, a large simulated dataset was created by coupling MATLAB and the chemical reactive-transport code HYTEC, considering the state-of-the-art GRAAL model (glass reactivity in allowance of the alteration layer). The trained models were then subsequently applied to the large-scale industrial, experimental data to identify potentially appropriate model parameters. Results indicate that ensemble methods can accurately predict viscosity as a function of temperature and composition across all three industrial datasets. Glass density prediction shows reliable learning performance with predictions primarily being within the experimental uncertainty of the test data. Furthermore, machine learning can predict glass dissolution model parameters behavior, demonstrating potential value in GRAAL model development and in assessing suitable model parameters for large-scale industrial glass dissolution data.

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