Models for Predicting the Viscosity of Nuclear Waste Glass Melts

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Nuclear waste vitrication in the UK sees a radioactive waste calcine combined with a borosilicate glass frit, and mixed in an induction melter at temperatures typically up to 1300 K before transfer to containers for storage and eventual disposal. Viscosity is a critical process parameter in this operation; too high and the melt will not mix or pour correctly into the containers, too low and the temperature can lead to volatilisation or the generation of unwanted refractory oxides. Understanding the effects of compositional changes on viscosity is therefore important in predicting melter operations. However, direct viscometry testing of all of these glasses is impractical on account of their radioactivity, inventory and uncertainty due to changing compositions as plants are being decommissioned. Here we describe how we have applied modelling and simulation to develop models to predict viscosity in these materials. The approach taken has been to utilise modelling and simulation across different length and time-scales in order to predict viscosity and understand the implications for plant performance. In the first part we will describe how we have utilised experimental data for inactive simulant nuclear waste glasses supplemented by the theoretical modelling semi-empirical, to predict the temperature-viscosity behaviour of different melts, including the data fitting methodology and model validation. In the second part we will describe how we have tested a molecule dynamics approach to calculating these properties from first principles, and describe the challenges and successes from computational and a physical model perspective. This work includes an assessment of equilibrium and non-equilibrium simulation approaches to calculate viscosity and a critical review of the empirical potential literature for borosilicate glasses. Finally we will describe how we are utilising this data in CFD models of the process.