Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.34514

Uncertainty Evaluation and Calibration in Neural Network Models for Melt Viscosity

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Melt viscosity is a key physical property in numerical simulations of heat and mass transport in volcanic magmas and glass-melting furnaces. Its nonlinear dependence on temperature and chemical composition makes theoretical prediction challenging. Although neural network–based models using chemical compositions have recently been proposed [1], quantitative evaluation of prediction uncertainty remains limited. In this study, we employ Monte Carlo (MC) dropout, a simple and computationally efficient approach for estimating model uncertainty [2], and examine the effects of hyperparameters and uncertainty calibration on predictive performance.

Using viscosity data for the SiO_2–Al_2O_3–MgO–CaO–Na_2O system (N = 4335), we developed a neural network model incorporating dropout. The target viscosity is expressed as $\log_{10}$ (η / Pa s), ranging from -1 to 13. Numerical experiments show that MC dropout captures prediction uncertainty consistent with variations in input chemical composition. However, the magnitude of the estimated uncertainty is highly sensitive to the dropout rate. In particular, with a commonly used dropout rate of 20%, the uncertainty was overestimated, reaching up to ±2 log units in the high-viscosity range.

We adopted a simple linear calibration originally proposed for post-hoc ensemble calibration [3]. By comparing the predicted uncertainty with the root-mean-square (RMS) of the actual prediction errors, the uncertainty estimates prior to calibration were systematically over- or underestimated depending on the dropout rate. After calibration, the predicted uncertainties were rescaled to an appropriate magnitude, resulting in improved consistency with the actual prediction errors. Overall, these results highlight the importance of evaluating and calibrating predicted uncertainties.

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