Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.37913

Model comparison and uncertainty estimation in amphibole thermobarometry using random forest and generalized additive models

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Magma storage pressures (*P*) and temperatures (*T*) are key intensive parameters for understanding the geometry and evolution of magmatic systems. These conditions are recorded in the chemical composition of minerals formed at depth, which can be transformed into quantitative estimates of *P* and *T* using thermobarometric models.

In recent years, single-phase thermobarometric models have been successfully calibrated using machine learning techniques (e.g., Random Forest), with the advantage of being widely applicable and not requiring a mineral or melt pair. Typically, the performance of these models is evaluated using metrics such as the root mean squared error (RMSE) on test datasets. Although these metrics are important for assessing overall model performance, they do not provide the uncertainty associated with individual predictions conditional on the covariates. However, such information is essential for interpreting thermobarometric results and addressing geological questions.

While estimating prediction uncertainty can be challenging for machine learning models such as Random Forest, the use of models with well-established statistical properties and comparable predictive performance in many scenarios, such as generalized additive models (GAM), enables the estimation of confidence intervals for individual predictions. Using a newly compiled experimental dataset (>1,200 amphibole–melt pairs), we find that the performance of Random Forest and GAM is comparable. We apply GAM (i.e. with uncertainty associated with each prediction), across the different eruptive periods of Mount St. Helens' last eruptive stage (Spirit Lake, 4 ka-present) to trace the temporal evolution of the plumbing system of this emblematic volcano. The thermobarometric calculations evidence the progressive thermal maturation of the magmatic system beneath Mount St. Helens during the last 4,000 years.