

# Plagioclase-Saturated Melt Hygrothermobarometry and Plagioclase-Melt Equilibria Using Machine Learning

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## RESEARCH ARTICLE

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Plagioclase-Saturated Melt Hygrothermobarometry and  
Plagioclase-Melt Equilibria Using Machine LearningK. S. Cutler<sup>1</sup> , M. Cassidy<sup>1,2</sup> , and J. D. Blundy<sup>1</sup> <sup>1</sup>Department of Earth Sciences, University of Oxford, Oxford, UK, <sup>2</sup>School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, UK

## Key Points:

- Investigation into whether existing plagioclase-based hygrothermobarometers can be refined using random forest machine learning
- The algorithm highlights that only melt composition is required to estimate intensive variables (P-T-H<sub>2</sub>O) of plagioclase-saturated magmas
- New melt models show improvement in errors compared to thermodynamic-based plagioclase-melt hygrothermobarometers and equilibria models

## Supporting Information:

Supporting Information may be found in the online version of this article.

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**Software:** K. S. Cutler  
**Supervision:** M. Cassidy, J. D. Blundy  
**Visualization:** K. S. Cutler  
**Writing – original draft:** K. S. Cutler  
**Writing – review & editing:** M. Cassidy, J. D. Blundy

**Abstract** Compositions of plagioclase-melt pairs are commonly used to constrain temperatures (T), dissolved water contents (H<sub>2</sub>O) and pressures (P) of pre-eruptive magma storage and transport. However, previous plagioclase-based thermometers, hygrometers, and barometers can have significant errors, leading to imprecise reconstructions of conditions during plagioclase growth. Here, we explore whether we can refine existing plagioclase-based hygrothermobarometers with either plagioclase-melt or melt-only chemistry ( $\pm T/H_2O$ ), calibrated using random forest machine learning on experimental petrology data ( $n = 1,152$ ). We find that both the plagioclase-melt and melt-only models return similar cross-validation root-mean-square errors (RMSEs), as the melt holds most of the P-T-H<sub>2</sub>O information rather than the plagioclase. T/H<sub>2</sub>O-dependent melt models have test set RMSEs of 25°C, 0.70 wt.% and 76 MPa for temperature, H<sub>2</sub>O content and pressure, respectively, while T/H<sub>2</sub>O-independent models have RMSEs of 38°C, 0.97 wt.% and 91 MPa. The melt thermometer and hygrometer are applicable to a wide range of plagioclase-bearing melts at temperatures between 664 and 1355°C, and with H<sub>2</sub>O concentrations up to 11.2 wt.%, while the melt barometer is suitable for pressures of  $\leq 500$  MPa. An updated plagioclase-melt equilibrium model has also been calibrated, allowing the equilibrium anorthite content to be predicted with an error of 5.8 mol%. The new P-T-H<sub>2</sub>O-An models were applied to matrix glasses and melt inclusions from the 1980 Mount St Helens (USA) and 2014–2015 Holuhraun (Iceland) eruptions, corroborating previous independent estimates and observations. Models are available at <https://github.com/kyra-cutler/Plag-saturated-melt-P-T-H2O-An>, enabling assessment of plagioclase-melt equilibrium and characterization of last-equilibrated P-T-H<sub>2</sub>O conditions of plagioclase-saturated magmas.

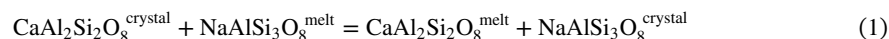
**Plain Language Summary** Thermobarometry and hygrometry are common methods for reconstructing magma crystallization conditions (pressure (P), temperature (T) and dissolved water content (H<sub>2</sub>O)) prior to eruption. Plagioclase is a ubiquitous mineral found in a wide range of volcanic rocks and is often used to estimate P-T-H<sub>2</sub>O conditions. Here, we use machine learning-based regression to calibrate new models, based on either plagioclase-melt or melt-only chemistry, to test whether we can improve the existing range of plagioclase-based thermobarometers and hygrometers. We also develop an updated model to determine the equilibrium composition of a plagioclase crystal with a given normalized melt composition. We find that the plagioclase-melt and melt-only thermobarometers and hygrometers return very similar model errors due to the melt holding nearly all the P-T-H<sub>2</sub>O information. The models can be applied to a wide range of plagioclase-bearing melts except for the barometer, which is only appropriate for upper crustal pressures of  $\leq 500$  MPa ( $\leq 13.8$  km depth). Models are available at <https://github.com/kyra-cutler/Plag-saturated-melt-P-T-H2O-An>, enabling assessment of plagioclase-melt equilibrium and characterization of last-equilibrated P-T-H<sub>2</sub>O conditions of plagioclase-saturated magmas.

## 1. Introduction

Temperature (T), pressure (P) and melt water contents (H<sub>2</sub>O) collectively control various physiochemical properties of magmas by influencing the crystallization and stability of mineral phases (e.g., Feig et al., 2010; Krawczynski et al., 2012), as well as the density and viscosity of melts (e.g., Giordano et al., 2008). Placing constraints on the thermal state, volatile concentration, and depths of magma crystallization thereby enables a critical insight into pre-eruptive storage conditions and magma transport properties, informing our understanding of controls on eruption dynamics and the crustal architecture of sub-volcanic systems (e.g., Bamber et al., 2022; Cassidy et al., 2018; Caricchi et al., 2021; Giordano & Caricchi, 2022). Furthermore, integrating petrological constraints with potential signs of volcanic unrest (i.e., seismicity, surface deformation, gas emissions; e.g.,

Cassidy et al., 2019; Liu et al., 2020; Saunders et al., 2012; Stock et al., 2018; Yip et al., 2022) can facilitate monitoring and hazard management at restless volcanoes (e.g., Pritchard et al., 2019).

Plagioclase is an abundant mineral found in volcanic rocks across a wide compositional range, with its chemistry sensitive to temperature, melt composition—including water content—and pressure (e.g., Housh & Luhr, 1991; Lange et al., 2009; Longhi et al., 1993; Namur et al., 2012; Panjasawatong et al., 1995). This has led to the development of a range of plagioclase-melt thermometers, hygrometers and barometers (e.g., Lange et al., 2009; Masotta & Mollo, 2019; Putirka, 2005, 2008; Waters & Lange, 2015), with expressions based on the equilibrium exchange of albite (Ab; NaAlSi<sub>3</sub>O<sub>8</sub>) and anorthite (An; CaAl<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>) components between plagioclase and melt (Equation 1):



Temperature and melt water contents recovered with plagioclase-melt thermometers and hygrometers have relatively small errors (e.g., Equation 24a, ±36°C; Putirka, 2008; ±0.29 wt.% (trachyte-specific) Masotta & Mollo, 2019; 0.35 wt.%, Waters & Lange, 2015; 1.1 wt.%, Putirka, 2008 (Equation 25b)), although such models are dependent on at least one independently constrained intensive variable (i.e., T, H<sub>2</sub>O or P), yielding higher errors when errors are propagated or iterative calculations are performed (Wieser, Gleeson, et al., 2023). The only plagioclase-melt barometer available is a formulation by Putirka (2005, 2008), which returns a significantly large Standard Error Estimate (SEE: 380 MPa; which is equivalent to ±10.5 km depth uncertainty using a 2700 kg/m<sup>3</sup> crustal density), resulting from the negligible volume change of reaction Equation 1 at low pressures (cf. ≤300 MPa; Lange et al., 2009). Similarly, other mineral-based barometer calibrations are associated with comparably poor accuracy and precision (e.g., clinopyroxene: 200–500 MPa, ±5.5–14 km depth, Wieser, Kent, & Till, 2023; amphibole: 300–400 MPa, ±8–11 km, Putirka, 2016), sufficient only for outlining broad depth ranges of magma crystallization. Establishing a precise and accurate barometer is thus a key petrological target for obtaining high-resolution images of magmatic systems, as identified by the SZ4 initiative (Hilley et al., 2022). The poor performance prevalent in the current scope of barometers may derive from various factors, including low precision electron microprobe measurements on pressure-sensitive analytes (i.e., Na<sub>2</sub>O in clinopyroxene; Wieser, Kent, & Till, 2023), disequilibrium textures in experimental products (e.g., clinopyroxene sector zoning; Neave and Putirka (2017)), or a weak pressure dependency on compositional variables (e.g., Putirka, 2016). Another factor that can contribute to the large uncertainty of pressure estimates is the strategy used to calibrate barometric models (Higgins et al., 2022). Recently, supervised machine learning (ML) algorithms have proven to be a successful approach to obtain T and P predictions (e.g., Higgins et al., 2022; Jorgenson et al., 2022; Petrelli et al., 2020; Thomson et al., 2021), as the algorithms are not reliant on any a priori thermodynamic knowledge and can capture non-linearity between variables.

Over the past 50 years, several empirical or thermodynamic-based models have been developed to predict the equilibrium compositions of plagioclase (An = [molar Ca/(Ca + Na + K)]) crystallizing from silicate melts. Although the majority of plagioclase-melt equilibria models primarily examine the effect of H<sub>2</sub>O and pressure on plagioclase composition (e.g., Housh & Luhr, 1991; Panjasawatong et al., 1995), limited studies have focussed on anhydrous systems or combined (hydrous and anhydrous) datasets (e.g., Fuhrman & Lindsley, 1988; Namur et al., 2012; Putirka, 2005). This necessitates creating an updated plagioclase-melt equilibria model applicable to modeling an extensive range of differentiated liquids irrespective of melt water content.

In this study, our aims are two-fold. With the large number of plagioclase-bearing experiments available, we first use machine learning (ML) to test whether we can refine the existing range (i.e., Putirka, 2005; Putirka, 2008; Waters & Lange, 2015; Masotta & Mollo, 2019) of plagioclase-based hygrometers either by using plagioclase-melt or melt-only chemistry. Second, we aim to create an ML model for predicting equilibrium plagioclase composition solely as a function of melt chemistry. We then test the capability of the models to recover magma crystallization conditions in two well-studied volcanic systems, comparing P-T-H<sub>2</sub>O-An estimates with melt inclusion analyses, geophysical data, and independent hygrometric and plagioclase-melt equilibria calculations.

## 2. Developing Hygrothermobarometric and Anorthite Content Models

### 2.1. Data Set Compilation and Filtering

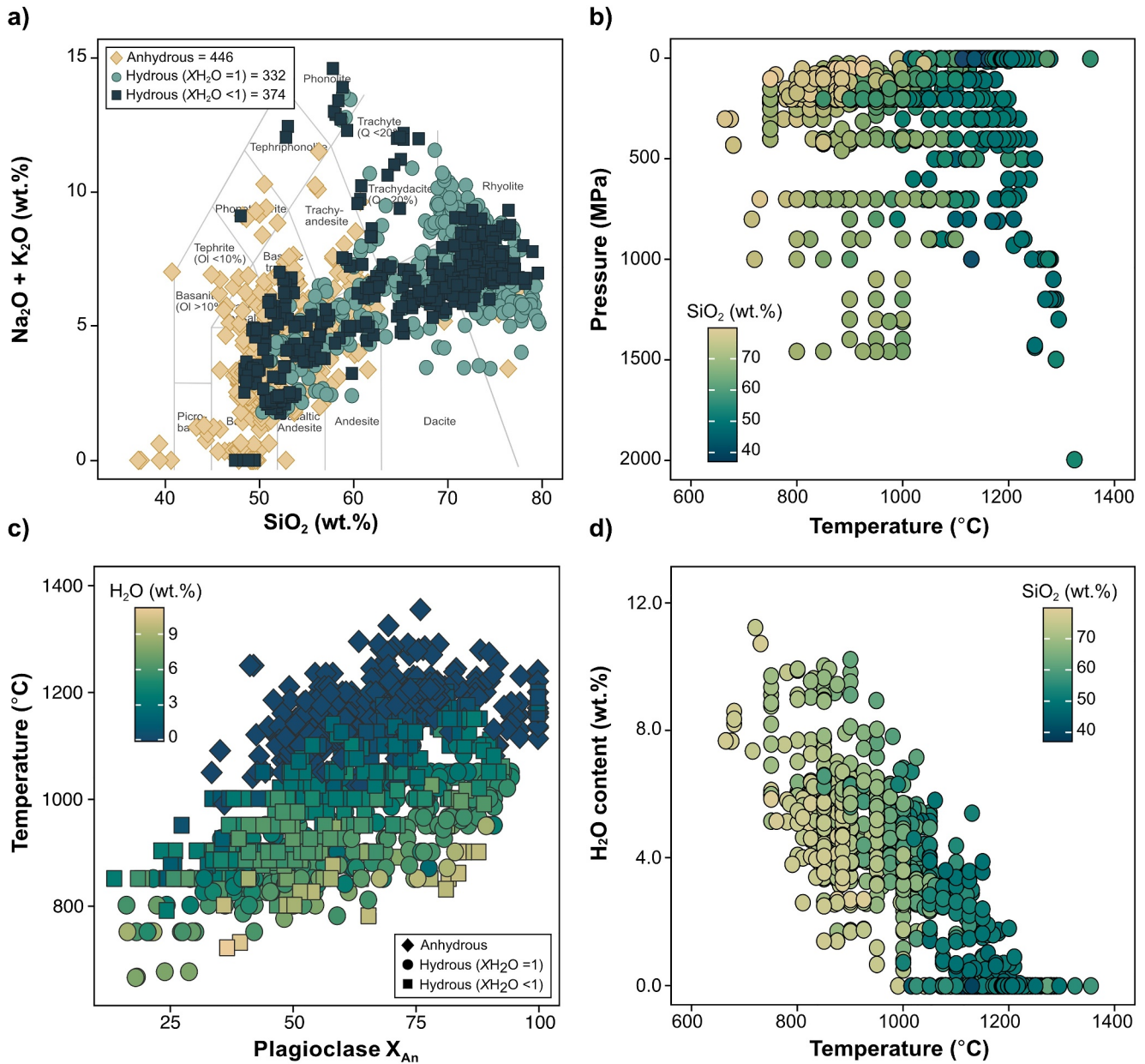
Experimental plagioclase-melt pairs were extracted from the Library of Experimental Phase Relations (LEPR) database (Hirschmann et al., 2008) and supplemented by an extensive literature search to calibrate all plagioclase-melt and melt-only versions of models. The final dataset ( $n = 1,152$ ) includes anhydrous/nominally anhydrous, fluid-saturated and fluid-undersaturated experiments; the full calibration dataset can be accessed in Table S1 in Supporting Information S2. We applied a set of filters to the experimental data to ensure coexisting plagioclase-melt pairs were in equilibrium (e.g., Lange et al., 2009; Namur et al., 2012; Waters & Lange, 2015): (a) only experiments with a quenched liquid (i.e., glass) fraction of  $\geq 50\%$  were selected, as high crystallinity charges are subject to slower diffusion rates in minerals compared to the melt, requiring longer timescales to reach equilibrium. Experiments were excluded if phase or crystallinity proportions were not reported. (b) Only experiments with electron microprobe analytical totals between 97 and 101.5 wt.% (including H<sub>2</sub>O) were incorporated. This filter ensures that any potential analytical errors are minimized. (c) Experiments were removed if papers reported evidence for significant sodium and/or iron loss ( $\geq 10$  wt.% relative Na<sub>2</sub>O or FeO). It must be noted that some plagioclase-saturated melt compositions in the literature lack compositions of coexisting plagioclases. For the hygrometry models, only experiments with well-constrained water analyses (i.e., Fourier-Transform InfraRed spectroscopy, Secondary Ion Mass Spectroscopy, Raman spectroscopy) were used as the water content values for calibration. However, only  $\sim 35\%$  of hydrous experiments have measured water content estimates. Therefore, MagmaSat (Ghiorso & Gualda, 2015) in VESICAL (Iacovino et al., 2021) was used to calculate the water content in the remaining water-saturated and undersaturated (if fluid XH<sub>2</sub>O value was reported) experiments.

### 2.2. Calibration Range

The calibration dataset covers a range of terrestrial and non-terrestrial analog melts (SiO<sub>2</sub>: 37.1–79.9 wt.%; Na<sub>2</sub>O + K<sub>2</sub>O: 0.3–14.6 wt.%) that crystallized plagioclase (An<sub>16–100</sub>) at conditions from 0 to 2000 MPa, 664–1355°C, and H<sub>2</sub>O concentrations up to 11.2 wt.% (Figure 1). Temperature displays a bimodal distribution with peaks at 850–900°C (felsic melts) and 1100–1200°C (mafic melts), whereas plagioclase compositions are symmetrically distributed. Pressure and H<sub>2</sub>O have strong positively skewed distributions. Excluding the experiments undertaken at 1 atm, 85% of the experiments occur at pressures of  $\leq 500$  MPa. There is minimal variation in T and H<sub>2</sub>O at pressures  $> 500$  MPa within the overall P range except for the 700 MPa experiments (Figure 1b). From all the hydrous experimental data, there is an evident lack of experiments with higher H<sub>2</sub>O ( $> 7$  wt.%) contents, although  $9 \pm 1$  wt.% represents the maximum limit to which H<sub>2</sub>O in experimental mafic melts can be quenched to glass (Gavrilenko et al., 2019). Experiments with lower H<sub>2</sub>O ( $< 2$  wt.%) are also underrepresented, reflecting limited studies that measure water content in near-anhydrous experimental glasses (i.e., Whittaker et al., 2007; Husen et al., 2016) and/or undertaking water-saturated runs at low pressures.

### 2.3. Model Training and Cross-Validation

A type of random forest machine learning algorithm, Extremely Randomized Trees, was used to train all the models using the package “ranger” and the *splitrule* “extratrees” (Wright & Ziegler, 2017) in R (R Core Team, 2013), as it has been shown to have the highest predictive capability among a selection of supervised learning algorithms (e.g., Li & Zhang, 2022; Petrelli et al., 2020). In short, random forest algorithms are an ensemble machine learning approach involving multiple decision trees, where the output of all individual trees is aggregated to form an averaged prediction. Each target variable (P-T-H<sub>2</sub>O-An) is predicted using normalized major element oxide compositions as dependent variables (melt: SiO<sub>2</sub>, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, FeO, MgO, CaO, Na<sub>2</sub>O, K<sub>2</sub>O; plagioclase: SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, FeO, CaO, Na<sub>2</sub>O, K<sub>2</sub>O) for the plagioclase-melt or melt-only models. MnO in the melt and MnO, TiO<sub>2</sub> and MgO in plagioclase were not considered as input variables since numerous experiments do not report one or more of these oxides and since they are uniformly at very low concentrations in plagioclase. The whole dataset was split into training and testing sets using an 80/20 ratio, with the test set held back and never used during model calibration. The training/testing sets were split using a stratified sampling function to ensure a balanced distribution of the models' target variable (i.e., H<sub>2</sub>O, temperature, pressure and An content) in both the training and testing sets. Models can be optimized by tuning hyperparameters, but studies have shown that it has little impact on model performance (e.g., Jorgenson et al., 2022; Petrelli et al., 2020). Therefore, we used the default hyperparameter tuning (i.e., *mtry*) within the Caret package (Kuhn, 2008) to optimize each model while

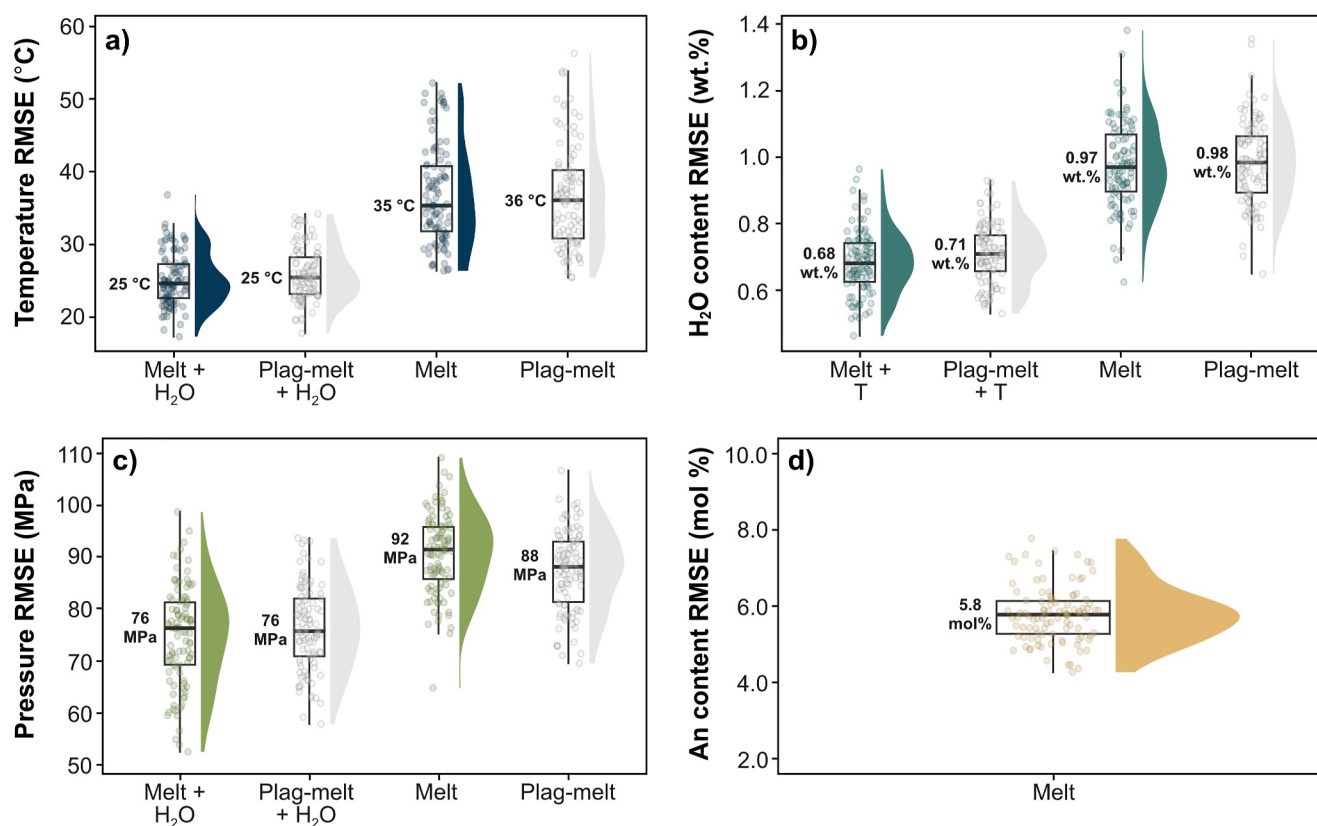


**Figure 1.** Calibration range of compiled plagioclase-saturated experiments. (a) Total alkali versus silica classification diagram after Le Maitre et al. (1989) of experimental glass compositions ( $n = 1152$ ). The anhydrous experimental total includes nominally anhydrous experiments ( $n = 17$ ). (b) Temperature (°C) versus pressure (MPa) of experiments. Color coding indicates SiO<sub>2</sub> (wt.%) of the melt. (c) Plagioclase composition in terms of temperature for all experimental data with plagioclase-melt compositions ( $n = 1063$ ) with color coding highlighting melt H<sub>2</sub>O (wt.%) content. (d) H<sub>2</sub>O (wt.%) versus temperature (°C) of experiments. Color coding reflects SiO<sub>2</sub> (wt.%) of the melt.

keeping the number of the decision trees small ( $num.trees = 200$ ) to minimize computational time. We use the median to average the final prediction from the 200 individual decision trees (Figure S1a in Supporting Information S1), which has been shown to return slightly lower RMSEs (Root Mean Square Errors) than the mean (Jorgenson et al., 2022; Weber & Blundy, 2024).

Model errors were assessed using two approaches. First, stratified 10-fold cross-validation was used on the training set using the Caret package, where the training set was split into 10 subsets or folds (Figure S1b in Supporting Information S1). One of the folds is left out for testing, while the remainder is used to train the model. This process is repeated until all 10 rows of folds are processed, generating a median R<sup>2</sup> (coefficient of





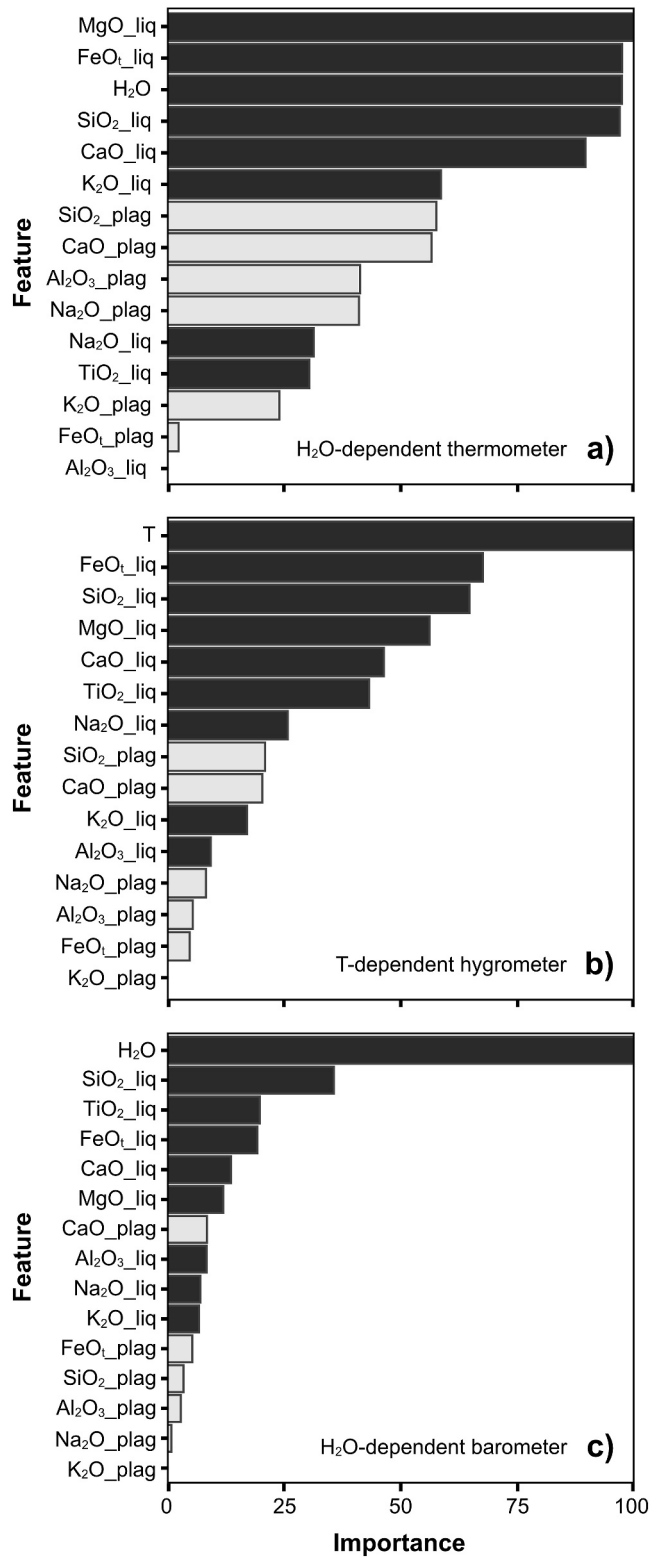
**Figure 2.** Raincloud comparison plots of cross-validation RMSEs from the plagioclase-melt and melt thermometer (a), hygrometer (b) and barometer (c) models as well as the plagioclase anorthite content model (d).

determination) and RMSE value. All folds were again stratified to remove an imbalanced distribution of the models' target variables. The models were also examined using the testing sets, providing independent metric values. The model RMSE and  $R^2$  values during cross-validation (CV) may differ slightly depending on how the training and testing sets are split. We thus repeated the workflow of random training/testing set splitting and 10-fold cross-validation 10 times (Figure S1b in Supporting Information S1). After model cross-validation and evaluation, the final saved models were trained on the full calibration dataset (i.e., Petrelli et al., 2020; Thomson et al., 2021).

### 3. P-T-H<sub>2</sub>O-An Models

#### 3.1. Model Calibration and Validation

Figure 2 highlights the overall variation and median RMSE values from the cross-validation of both plagioclase-melt and melt hydrothermobarometry models. The plagioclase-melt and melt models for each variable (P-T-H<sub>2</sub>O) depict a remarkably similar performance. The similarity across all models results from the predictive capability of the algorithm predominantly using the melt rather than the plagioclase compositional components (Figure 3), effectively rendering the plagioclase information redundant. This is unlike other random forest-calibrated models using mineral-melt pairs (clinopyroxene, Petrelli et al., 2020; biotite, Li & Zhang, 2022), where both the crystal and melt chemistry information improve the RMSE and  $R^2$  scores. The melt model RMSEs also reaffirm the utility of silicate melt composition in recovering key magmatic variables (e.g., Blundy, 2022; Helz & Thornber, 1987; Weber & Blundy, 2024; Yang et al., 1996). This finding results from the low thermodynamic variance of natural magmatic compositions whose overall chemical variability can be described with a relatively limited number of independent compositional variables, significantly fewer than the total number of constituent oxides, as determined using Principal Component Analysis (Weber & Blundy, 2024). In this section, we will thus focus on the melt models, which are appropriate for use with compositions of quenched and entrapped liquid (i.e., matrix glass or plagioclase-hosted melt inclusions). We will also examine limitations affecting model accuracy



**Figure 3.** Plots of variable importance versus input variable for the H<sub>2</sub>O-dependent thermometer (a), T-dependent hygrometer (b), and H<sub>2</sub>O-dependent barometer (c). All plots highlight the most important variables used by the algorithm to make predictions. Light gray bars represent plagioclase compositional inputs, and dark gray bars represent melt oxide inputs along with additional parameters such as T or H<sub>2</sub>O.

(i.e., model calibration) and precision (i.e., analytical uncertainties) to obtain P-T-H<sub>2</sub>O estimates and compositions of plagioclase.

### 3.2. Thermometry

Temperature and H<sub>2</sub>O in the experimental dataset display a strong inverse correlation (Figure 1d), leading us to test both H<sub>2</sub>O-independent and H<sub>2</sub>O-dependent thermometers. In both instances, the H<sub>2</sub>O-independent and H<sub>2</sub>O-dependent thermometers yield low mean cross-validation (H<sub>2</sub>O-independent, 35°C; H<sub>2</sub>O-dependent, 25°C; Figure 2) and test set RMSE values (H<sub>2</sub>O-independent, 38°C; H<sub>2</sub>O-dependent, 26°C). Systematic model errors were assessed by calculating the Mean Bias Error (MBE) as well as by checking the regression gradients and intercepts (Wieser, Gleeson, et al., 2023). Both thermometers have relatively low intercept and MBE values with high gradients close to 1 (Figures 4b and 5b), indicating no systematic offsets across the wide temperature range. Figures 4b and 5b display the test set residual distribution from all workflow replications and illustrate that 74% and 83% of residuals are within  $\pm 30^\circ\text{C}$  of the actual experimental temperature for the H<sub>2</sub>O-independent and H<sub>2</sub>O-dependent thermometers, respectively. The accuracy of the thermometers primarily results from the strong non-linearity of MgO, SiO<sub>2</sub>, FeO<sub>l</sub> and CaO in the melt when plotted against temperature (Figure S2 in Supporting Information S1). This is consistent with other liquid thermometers that prioritize MgO, FeO<sub>l</sub> and CaO within their parameterizations (e.g., Helz & Thornber, 1987). To further validate the ML models, we compare all our ML test set predictions (P-T-H<sub>2</sub>O-An) with estimates generated by previous hygrometric and plagioclase-melt equilibria models (Figure 6). We use Thermobar (version 1.011; Wieser, Petrelli, et al., 2023) to calculate estimates from previous models but limit ourselves to models calibrated for a wide compositional range to ensure comparison across similar experimental conditions. We only compare our H<sub>2</sub>O-dependent thermometer with the plagioclase-saturated liquid thermometer of Putirka (2008) (Equation 26; calibrated for T in the range 850–1350°C) as both models require H<sub>2</sub>O inputs. The ML H<sub>2</sub>O-dependent thermometer performs better than Equation 26 with a lower RMSE (26°C vs. 36°C), MBE (−0.94°C vs. −9.6°C) and intercept (41°C vs. 112°C) value as well as a gradient and R<sup>2</sup> value closer to 1 (Figures 5b and 6a).

### 3.3. Hygrometry

We tested a T-dependent (Figures 5c and 5d) and T-independent hygrometer (Figures 4c and 4d), as temperature is not always well-constrained in petrological studies. The T-dependent hygrometer (Figure 5c) returns median cross-validation and test set RMSE values of 0.68 wt.% and 0.69 wt.%, respectively, while the T-independent hygrometer (Figure 4c) gives reasonable cross-validation (0.97 wt.%) and test set (0.95 wt.%) RMSE scores. No systematic offsets across the range of H<sub>2</sub>O contents are apparent in the test data for both hygrometers, as they each have low intercept and MBE values and gradients close to 1 (Figures 4d and 5d). A closer look at the residuals, when grouped by type of experiment, reveals that the T-dependent hygrometer displays no difference in the modal and median values for anhydrous and hydrous ( $X_{\text{H}_2\text{O}} = 1$  and  $X_{\text{H}_2\text{O}} < 1$ ) experiments (Figure S3 in Supporting Information S1), with all groups concentrated at zero. For fluid-saturated experiments, the T-independent hygrometer residuals are centered at −1, indicating the model tends to slightly underestimate H<sub>2</sub>O compared to fluid-undersaturated and anhydrous experiments. Temperature is an important variable in predicting melt water content, with 70% of the residuals for the T-dependent hygrometer within  $\pm 0.5$  wt.% of the actual water content value (Figure 5d) compared to 58% of the residuals for the T-independent hygrometer (Figure 4d). Aside from temperature, FeO<sub>l</sub>, SiO<sub>2</sub>, and MgO play a key role in water content predictions, in which the algorithm appears to use these three oxides to characterize H<sub>2</sub>O content depending on the level of melt differentiation (Figure S4 in Supporting Information S1). These results broadly correspond with the findings of Zimmer et al. (2010), who show that an inverse correlation exists between the level of Fe enrichment in melts (i.e., tholeiitic index) and their water content. We use the Putirka (2008; calibrated for liquids with  $< 9$  wt.% H<sub>2</sub>O) and Waters and Lange (2015; calibrated for liquids with 0–8.3 wt.% H<sub>2</sub>O) plagioclase-melt hygrometers to make a comparison with the T-dependent hygrometer, as all models require temperature inputs. The T-dependent hygrometer outperforms the Putirka (2008) and Waters and Lange (2015) plagioclase-melt hygrometers with a lower overall RMSE (0.69 wt.%), MBE (−0.02 wt.%) and high gradient (0.94) and R<sup>2</sup> value (0.93; Figures 5d and 6b).



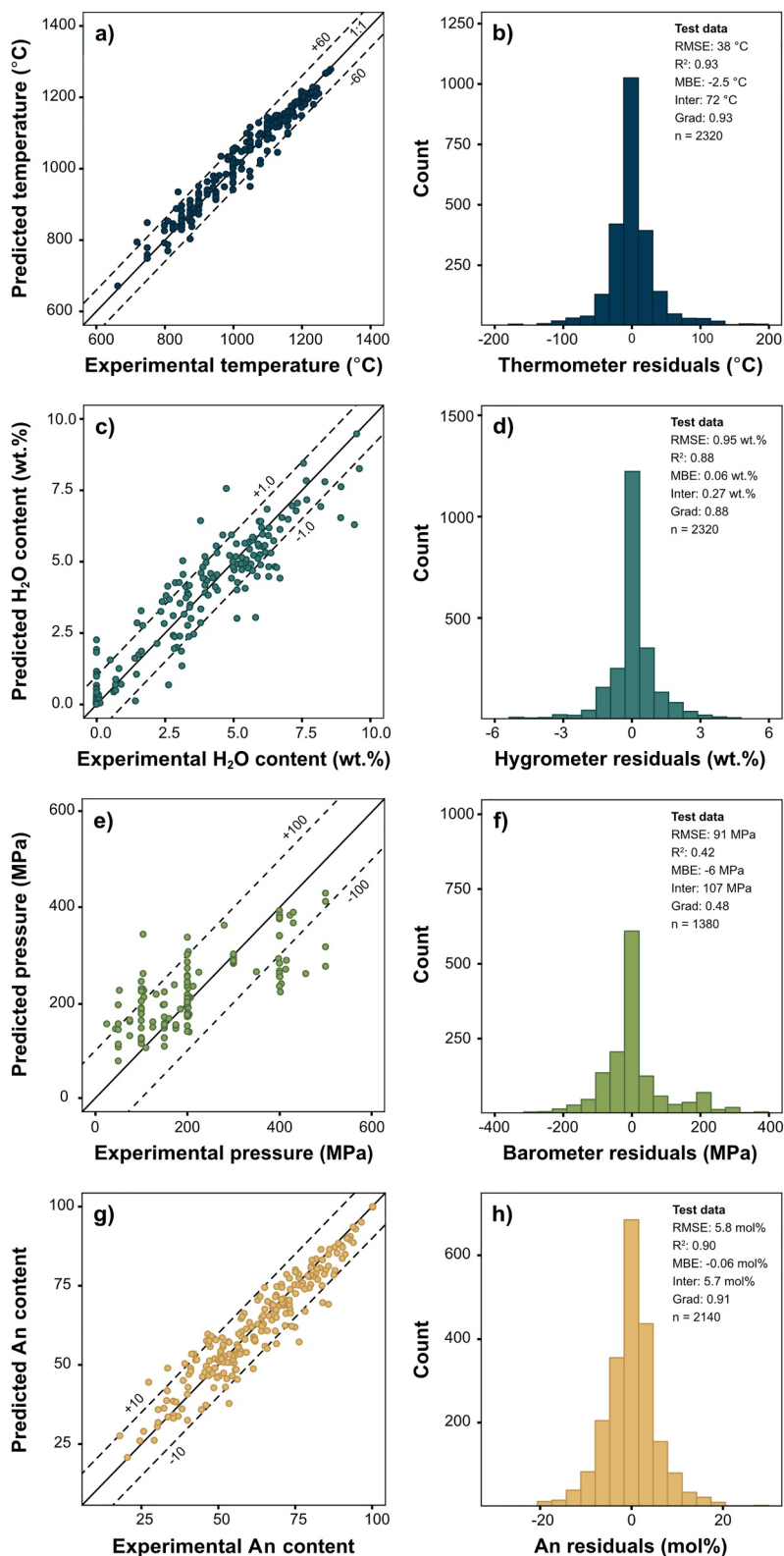


Figure 4.

### 3.4. Barometry

We tested an H<sub>2</sub>O-dependent (Figures 5e and 5f) and an H<sub>2</sub>O-independent barometer (Figures 4e and 4f), as H<sub>2</sub>O contents are not always well-constrained for natural systems, especially for lava lacking glassy melt inclusions suitable for direct H<sub>2</sub>O analysis. The barometers are calibrated using a reduced dataset by removing all high-pressure experiments (>500 MPa) due to the low number and narrow compositional range of experiments undertaken at higher pressures (Figure 1b). Atmospheric pressure experiments were also removed, as the pressure output for nominally anhydrous natural samples is likely to skew toward 0.1 MPa when H<sub>2</sub>O is used as an additional input variable. Both barometers perform surprisingly well with 10-fold cross-validation (H<sub>2</sub>O-dependent RMSE: 76 MPa; Figures 5e and 5f, H<sub>2</sub>O-independent RMSE: 92 MPa, Figures 4e and 4f), which is confirmed by their predictive performance in the test set (H<sub>2</sub>O-dependent RMSE: 76 MPa, H<sub>2</sub>O-independent RMSE: 91 MPa; Figures 4e and 5e), although the R<sup>2</sup> values for both barometers are low (H<sub>2</sub>O-dependent R<sup>2</sup>: 0.60; H<sub>2</sub>O-independent R<sup>2</sup>: 0.42; Table S2 in Supporting Information S1). In terms of residuals, the addition of H<sub>2</sub>O as an input enables 85% of the predictions to be within  $\pm 100$  MPa of the actual experimental pressure for the H<sub>2</sub>O-dependent barometer (Figure 5f) compared to 76% for the H<sub>2</sub>O-independent (Figure 4f) barometer. None of the melt components has a dominant control on the pressure predictions, where it would be expected that Al<sub>2</sub>O<sub>3</sub> and Na<sub>2</sub>O would correlate with pressure (Blundy, 2022). Instead, the algorithm mainly uses SiO<sub>2</sub>, TiO<sub>2</sub>, FeO, MgO and CaO, suggesting that, like the hygrometers, the extent of differentiation helps constrain pressure values in a hypothetical P-T(-H<sub>2</sub>O) space. The test set predictions for both barometers are systematically slightly offset as predictions <300 MPa tend to slightly overestimate pressures, while the barometers underestimate pressures >300 MPa, evident from the low gradient values and higher intercepts (Figures 4e and 5e). However, this pattern is similar to other barometers (e.g., clinopyroxene-based; Wieser, Gleeson, et al., 2023), likely amplified by the significant data gaps present at higher pressures in calibration datasets and the weak pressure trends with compositional variables. This highlights a crucial objective to conduct systematic experiments >300 MPa for a wide array of melt compositions to explore pressure correlations fully. To compare our H<sub>2</sub>O-dependent barometer performance, we use the Putirka (2008) plagioclase-liquid barometer (Equation 25a; calibrated for  $P < 2000$  MPa) because both barometers require an H<sub>2</sub>O input. A comparison of model performance statistics (Figures 5f and 6c) for the ML and plagioclase-liquid barometer highlights that the ML barometer represents a significant improvement in reducing pressure estimate errors.

### 3.5. Anorthite Content

We tested a model to estimate the composition of plagioclase (An content) as a function of the melt composition. The An model performs well without incorporating temperature and H<sub>2</sub>O as additional input variables (Figures 4g and 4h), with a median 5.8 mol% RMSE during cross-validation (Figure 2d) and a 5.8 mol% RMSE for the test set data (Figure 4g). The test data show no overall systematic offset across the An content range with low intercept and MBE values and a gradient close to 1 (Figure 4g), attesting to the model's high accuracy of anorthite predictions. Furthermore, 69% of the predictions have residuals within  $\pm 5$  mol% of the measured values and 91% within  $\pm 10$  mol%. CaO, SiO<sub>2</sub> and MgO in the melt are the dominant controls on plagioclase anorthite content (Figure S5 in Supporting Information S1), consistent with thermodynamic and experimental studies (e.g., Namur et al., 2012; Neave & Namur, 2022; Panjasawatong et al., 1995). With temperature exerting a primary control on plagioclase composition (e.g., Kudo & Weill, 1970; Lange et al., 2009; Figure 1c), the combination of CaO, SiO<sub>2</sub> and MgO also likely acts as an indirect proxy for temperature aiding anorthite predictions. We test our ML anorthite model against model E of Putirka (2005), calibrated on experiments with SiO<sub>2</sub> contents of 42–73 wt.% and plagioclase compositions of An<sub>40-95</sub> (Figure 6d). We also compare the anhydrous test set experiments with the T-independent models (Equations 33–35) of Namur et al. (2012) that are all calibrated on 0.1 MPa experiments with SiO<sub>2</sub> contents of 43–78 wt.% and plagioclase compositions of An<sub>39-100</sub>. The ability of the ML model to predict equilibrium plagioclase compositions is greater than that of model E (Figure 6d; e.g., RMSE: 14 mol%),

**Figure 4.** Examples of testing set performance for the melt-only models and residual (difference between experimental value and predicted value) histograms. Only the best-performing testing set is shown for each model. Testing set statistics in the histograms reflect the average RMSE, R<sup>2</sup>, MBE, intercept and gradient values across all 10 testing sets. (a) Comparison of experimental versus predicted temperature (°C) showing a 1:1 correspondence line. (b) Histogram for temperature residuals for all test sets. (c) Comparison of experimental versus predicted water content (wt.%). (d) Histogram of water content residuals for all test sets. (e) Comparison of experimental versus predicted pressure (MPa). (f) Histogram of pressure residuals for all test sets. (g) Comparison of experimental versus predicted anorthite content (mol%). (h) Histogram of anorthite content residuals for all test sets.

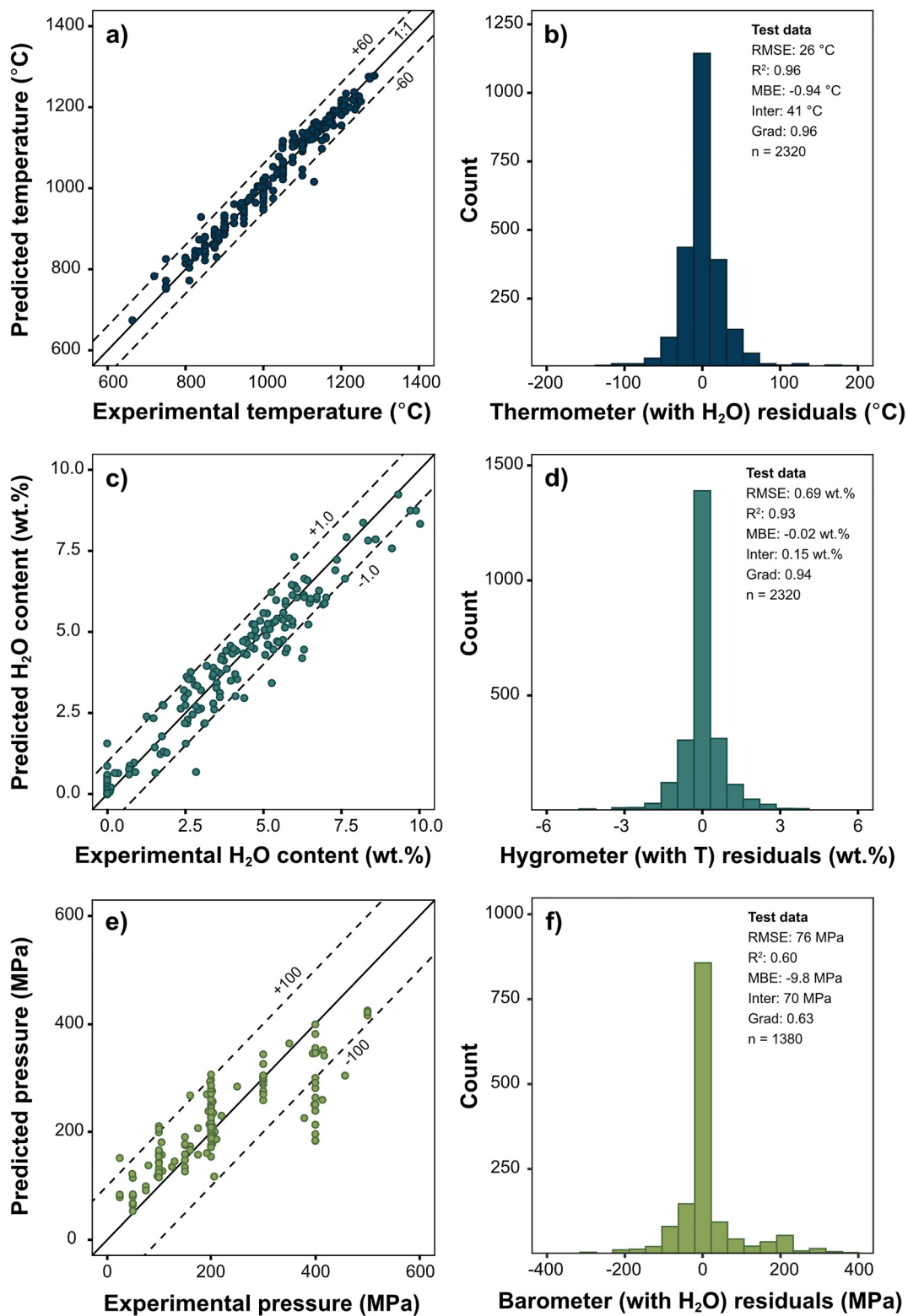


Figure 5.

whereas for the subset of anhydrous experiments, Namur et al.'s (2012) T-independent empirical models (Equations 33–35) have comparable RMSE, intercept and gradient values to the ML model, although the latter has a lower MBE and a higher  $R^2$  value (Figures 4h and 6d).

### 3.6. Plagioclase Saturation

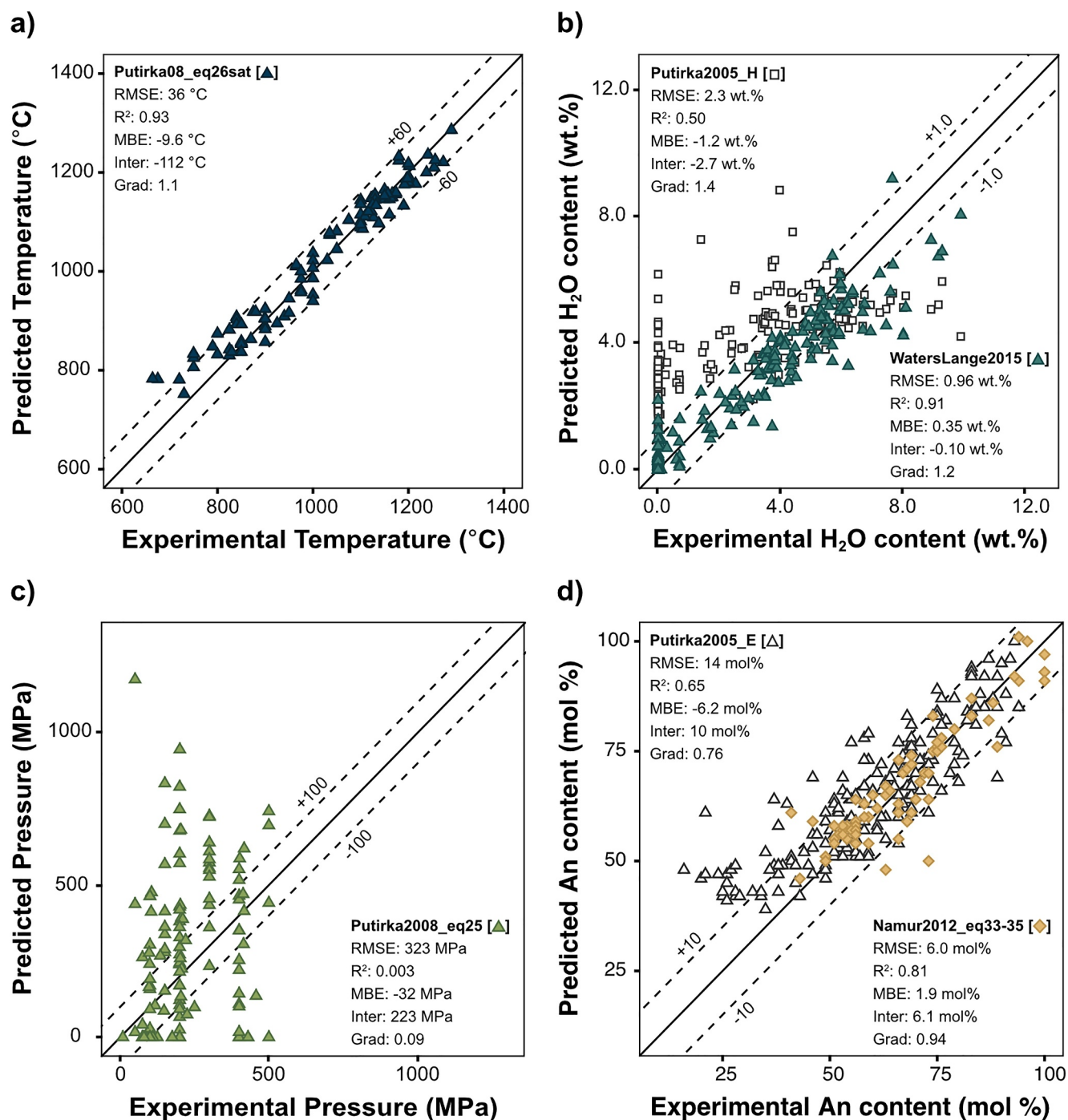
Before using any of the models, melt compositions must first be checked for plagioclase saturation to avoid erroneous model predictions, which may prove difficult if petrographic or microanalytical analyses cannot be carried out on samples, for example, in cases where only bulk rock data are available. We have thus developed a classifier model to screen matrix glass compositions for plagioclase saturation. We compiled an approximately equal amount of non-plagioclase to plagioclase-saturated experimental data ( $n_{\text{total}} = 2206$ ) for calibration (Table S3) and used the classification mode of the algorithm to train the model. The classifier cross-validation process is the same as all the regression models outlined in Section 2.2, but 5-fold cross-validation was used instead. We use the classification accuracy metric to evaluate the classifier's performance, which is a ratio describing the number of correct predictions to the total number of predictions. The mean accuracy from cross-validation and test sets is 87% and 90%, respectively. Table S4 in Supporting Information S1 presents an average test set confusion matrix, which summarizes all sets of classification results (i.e., false positive, false negative, true positive, true negative) from all test set replications and indicates low rates of false positive (~4%) and false negative (~5%) classifications.  $\text{SiO}_2$ ,  $\text{MgO}$ , and  $\text{Al}_2\text{O}_3$  are the main melt oxides used to classify plagioclase saturation, corresponding to  $\text{SiO}_2$  and  $\text{MgO}$  acting as differentiation and temperature proxies and  $\text{Al}_2\text{O}_3$  indicating the onset of plagioclase crystallization.

### 3.7. Further Model Limitations

The P-T- $\text{H}_2\text{O}$  bounds of the calibration dataset represent one major limitation of all models. The models presented here should *never* be used outside the calibration range since the ML algorithm is unsuitable for extrapolation. Additional experimental constraints covering key calibration dataset gaps will help to increase model accuracy (i.e., Figure 1). Furthermore, hygrometer RMSEs could be improved if more experimental glasses were analyzed for  $\text{H}_2\text{O}$  to increase the number of direct  $\text{H}_2\text{O}$  measurements within the calibration dataset, rather than using indirect  $\text{H}_2\text{O}$  estimates from solubility models (e.g., Ghiorso & Gualda, 2015; Papale et al., 2006; Zhang et al., 2007) or the 'volatiles by difference' method (e.g., Devine et al., 1995) that can have large uncertainties (e.g., Hughes et al., 2019). This is particularly true for low- $\text{H}_2\text{O}$  melts.

The precision of P-T- $\text{H}_2\text{O}$ -An predictions is influenced by the analytical error of the melt composition itself (e.g., Gualda & Ghiorso, 2014; Wieser, Kent, et al., 2023). To evaluate the impact of analytical (i.e., electron microprobe; EPMA) uncertainties on P-T- $\text{H}_2\text{O}$ -An predictions, we used a series of Monte Carlo simulations to create major element oxide variation based on 10 melt compositions (Table S5 in Supporting Information S3). These 10 melts were chosen to represent the compositional range and experimental conditions throughout the calibration dataset. For each melt, new compositions are generated from its original oxide values with noise added from a normal distribution, with the variation deriving from a weighted mean of one sigma standard deviation EPMA values (Table S5 in Supporting Information S3) from a subset of experiments ( $n = 400$ ). The 10 melts generated 2000 melt compositions by running a 200-time simulation per composition and subsequently used as inputs for each melt model. The simulations for the melt-only models highlight that analytical errors impose a limit on precision of  $\pm 44$  MPa for pressure,  $\pm 23^\circ\text{C}$  for temperature,  $\pm 0.56$  wt.% for  $\text{H}_2\text{O}$  (with temperature),  $\pm 0.88$  wt.% for  $\text{H}_2\text{O}$  (without temperature) and  $\pm 4.6$  mol % for anorthite content (Figures 7a–7g). In addition, analytical uncertainties associated with  $\text{H}_2\text{O}$  content inputs measured by SIMS or FTIR/Raman spectroscopy were also tested using a pessimistic averaged standard deviation of 0.5 wt.% (Ulmer et al., 2018), as few studies provide sufficient information (e.g., the number of analyses, standard deviations of water measurements) to calculate a reliable weighted mean. The simulations indicate that melt and water analytical errors can limit  $\text{H}_2\text{O}$ -

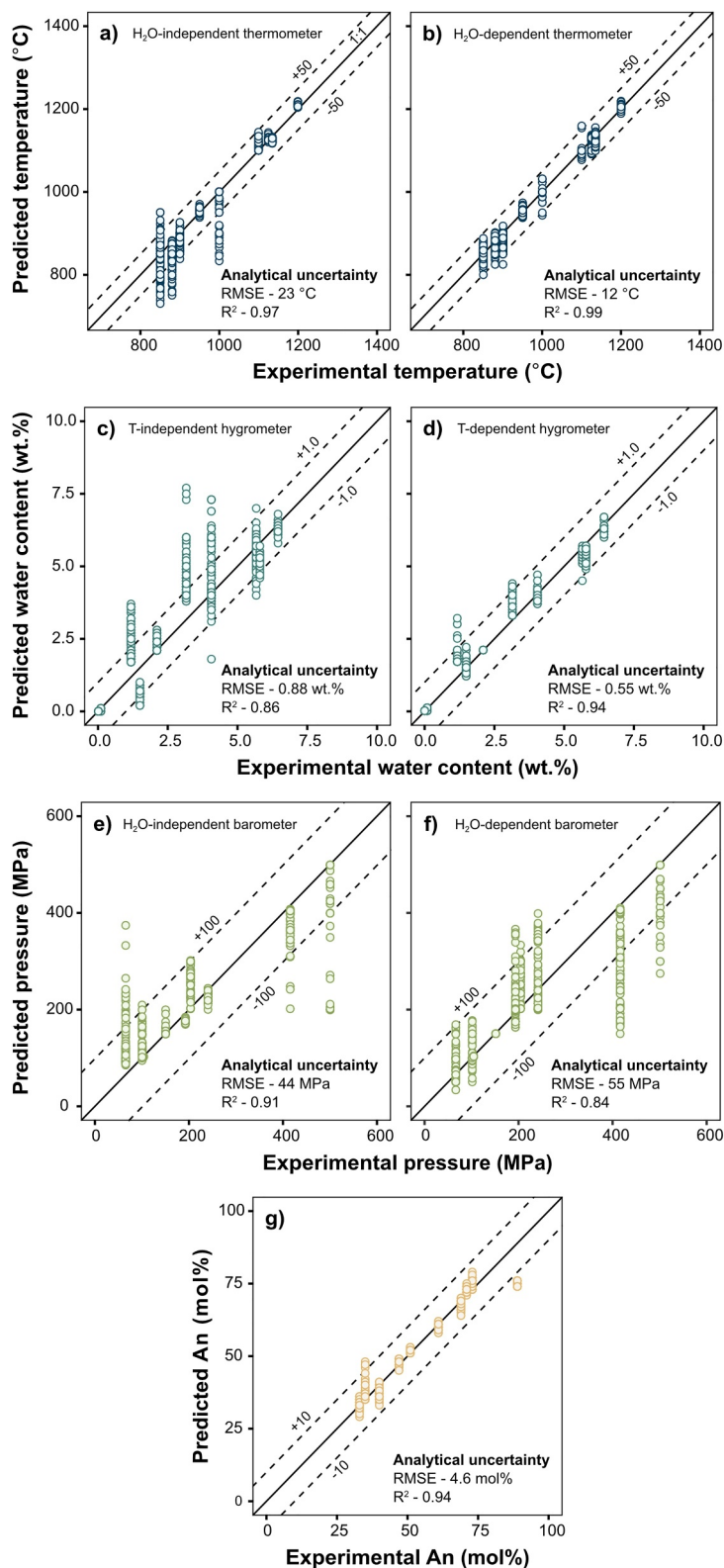
**Figure 5.** Examples of testing set performance for the melt models with additional input parameters (T or  $\text{H}_2\text{O}$ ) and residual histograms. Only the best-performing testing set is shown for each model. Testing set statistics in the histograms reflect the average RMSE,  $R^2$ , MBE, intercept and gradient values across all 10 testing sets. (a) Comparison of experimental versus predicted temperature ( $^\circ\text{C}$ ) using a 1:1 correspondence line. (b) Histogram for temperature residuals for all test sets. (c) Comparison of experimental versus predicted water content (wt.%). (d) Histogram of water content residuals for all test sets. (e) Comparison of experimental versus predicted pressure (MPa). (f) Histogram of pressure residuals for all test sets.



**Figure 6.** Testing set performance using other plagioclase-melt or melt models. Only the best-performing testing set is shown for each model, but the testing set statistics reflect the average RMSE, R<sup>2</sup>, MBE, intercept and gradient values across all 10 testing sets. (a) Plot of experimental temperature versus the predicted temperature (°C) derived from liquid thermometer (Equation 26) of Putirka (2008). (b) Plot of experimental water contents versus the predicted water contents (wt.%) resulting from plagioclase-melt hygrometers of Putirka (Model H; 2008) and Waters and Lange (2015). (c) Plot of experimental pressure versus the predicted pressure (MPa) resulting from the plagioclase-melt barometer (Equation 25) of Putirka (2008). (d) Plot of experimental anorthite content versus the predicted anorthite content (mol%) derived from the plagioclase-melt equilibria model of Putirka (Model E; 2008) and Namur et al. (Equations 33–35; 2012).

dependent model precision to  $\pm 55$  MPa for pressure and  $\pm 12^\circ\text{C}$  for temperature (Figures 7b and 7f). Both sets of simulations indicate the sensitivity of our hygrothermobarometers to analytical uncertainty. The simulations emphasize the need to undertake careful preparation (i.e., tephra extraction, Cooper et al., 2019; glass alteration





**Figure 7.** Monte Carlo simulations of electron microprobe analytical errors and their effect on the resulting temperatures (a, H<sub>2</sub>O-independent thermometer; b, H<sub>2</sub>O-dependent thermometer), water contents (c, T-independent hygrometer; d, T-dependent hygrometer), pressures (e, H<sub>2</sub>O-independent barometer; f, H<sub>2</sub>O-dependent barometer), and anorthite content estimates (g).

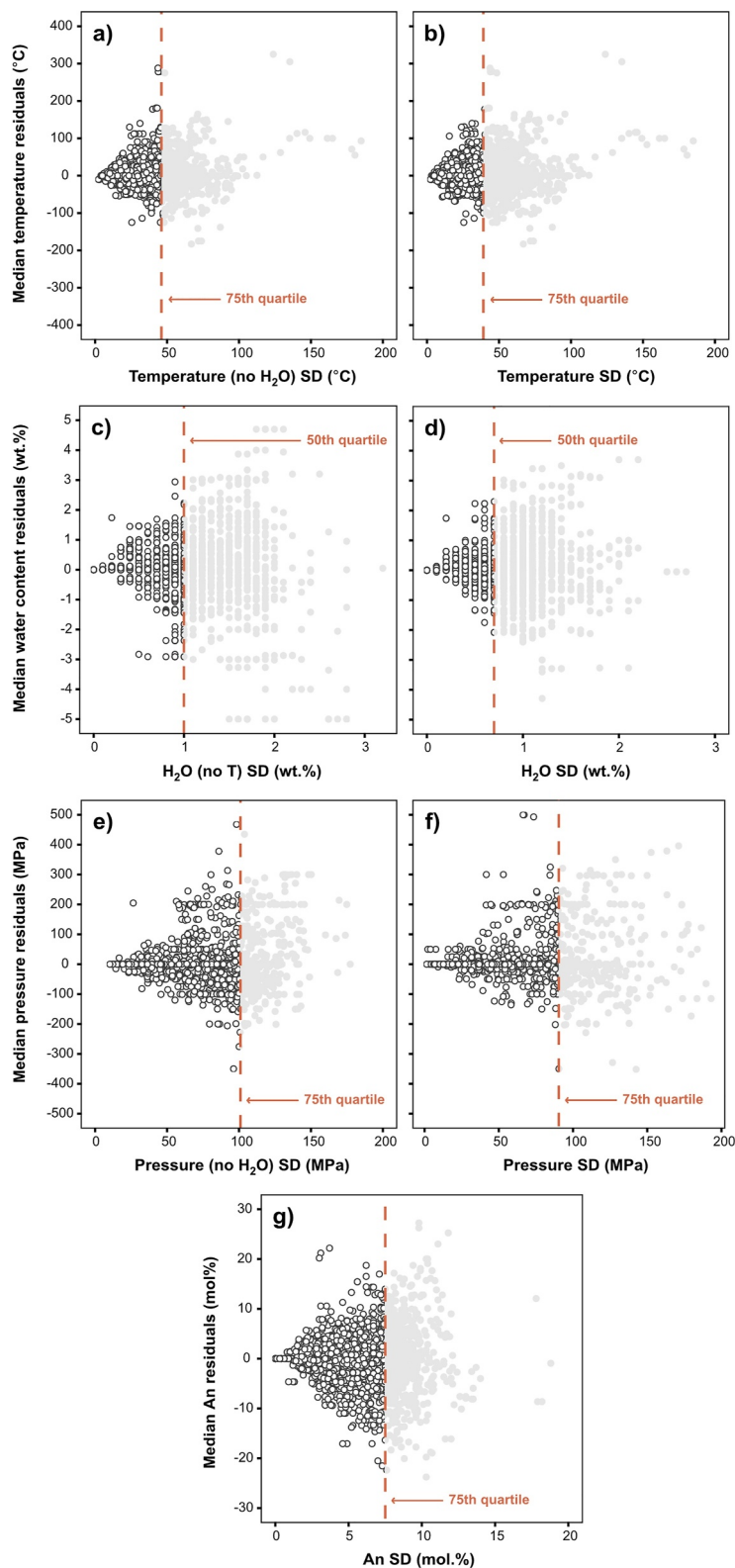


Figure 8.

recognition) and analytical procedures (i.e., EPMA; Hayward, 2012) of matrix glass and inclusions to minimize the chemical variability of susceptible oxides (e.g., MgO, SiO<sub>2</sub>) that would affect subsequent predictions.

#### 4. Model Application

To test the calibrations of our melt models, we have applied them to two tectonically contrasting, well-constrained volcanic systems (Mount St Helens, USA; Bárðarbunga, Iceland). We compare the predicted values to previous estimates calculated from various thermobarometers, direct H<sub>2</sub>O measurements from melt inclusions and seismic information about the sub-volcanic systems. For each application, we also discuss the different ways the models can be used depending on whether the melt H<sub>2</sub>O contents are known, along with suggestions on P-T-H<sub>2</sub>O-An and plagioclase saturation prediction filtering.

##### 4.1. May–October 1980 Eruption, Mount St Helens, USA

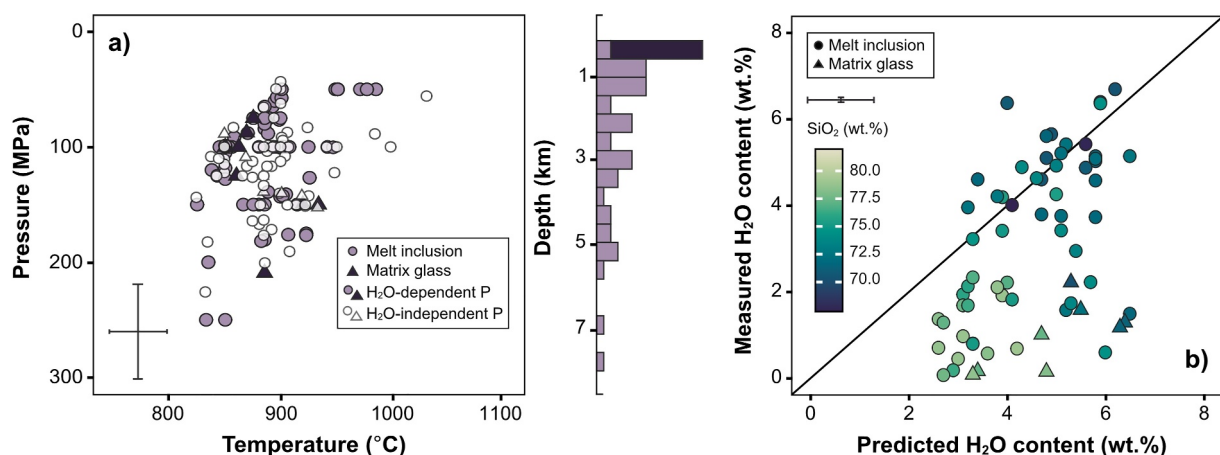
On 18 May 1980, the north flank of Mount St Helens' edifice collapsed, depressurizing the shallow magmatic “cryptodome” and triggering a lateral blast. Eruption of a 24 km high Plinian column ensued later that day as depressurization reached the deeper magmatic system. Smaller explosive eruptions characterize subsequent activity from May–October 1980; a series of dome-forming extrusions within the crater followed through to October 1986. Here, we apply the models to matrix glass and plagioclase-hosted melt inclusion data ( $n = 151$ ) in Blundy et al. (2008) from the 1980 eruptive activity of Mount St Helens. The erupted magma was a porphyritic dacite (or silicic andesite) with ~63 wt.% SiO<sub>2</sub> and ~35 vol% phenocrysts. The melt phase, both as inclusions and matrix glass, was uniformly rhyolitic and thought to be saturated in plagioclase, orthopyroxene, magnetite and ilmenite (Rutherford et al., 1985). Amphibole also occurs as a phenocryst phase but shows some evidence of resorption or breakdown, notably in the dome-forming magmas. Clinopyroxene is a rare phenocryst phase in some samples.

In cases where constraints for all variables (P-T-H<sub>2</sub>O-An) are unknown, the variables should be recovered sequentially in the following order: An → T → H<sub>2</sub>O → P (Figure S6 in Supporting Information S1). Before using the P-T-H<sub>2</sub>O models, glass compositions must demonstrate that they represent a melt in equilibrium with plagioclase, which can be achieved by comparing An predictions from the plagioclase-equilibria model with natural plagioclase rim compositions. The uncertainty of a prediction is given as the standard deviation and can be used to filter model predictions to further reduce errors. This has been shown by Weber and Blundy (2024), where their model test set predictions using a random forest algorithm display higher residual variance as the standard deviation (SD) increases. Figure 8 presents our melt model test set residuals against the SD and shows that most of the divergence begins from the 75th quartile of SD values. In addition, our test set statistics display an improvement with overall lower RMSE, intercept, and MBE values with higher gradients and R<sup>2</sup> values, especially in the case of the barometers (Figures 8e and 8f). Therefore, we recommend filtering values by removing the top 25% SD values. However, for the hygrometers, removing values above the 50th quartile is more effective at reducing the variance (Figure 8). Although filtering will lead to fewer predictions, removing predictions with the highest variance will ensure more robust estimates. Accordingly, we only report the filtered estimates from all models with both applications (Table S6).

The range of plagioclase compositions in equilibrium with the compositional range of plagioclase-hosted melt inclusions and matrix glasses is estimated at An<sub>21-51</sub> (matrix mode: 45 mol%; MI mode: 39 mol%), which corresponds within error to the dominant plagioclase rim composition (An<sub>47</sub>; Berlo et al., 2007), suggesting that the plagioclase rims were in equilibrium with the host melt.

The H<sub>2</sub>O-independent thermometer returns mean melt inclusion and matrix glass temperatures of 892 ± 55°C (SD) and 885 ± 49°C (Figure 9a), respectively; the former is consistent with melt inclusion temperatures (853–

**Figure 8.** Investigation of appropriate filters for all testing set P-T-H<sub>2</sub>O-An estimates using the standard deviation. Dashed lines highlight the 50th or 75th standard deviation quartile, where estimates (light gray points) greater than this value should be removed. The testing set statistics reflect the average RSME, R<sup>2</sup>, MBE, intercept and gradient values across all 10 testing sets after filtering. (a) Median temperature residuals versus temperature SD (°C) for the H<sub>2</sub>O-independent thermometer. (b) Median temperature residuals versus temperature SD (°C) for the H<sub>2</sub>O-dependent thermometer. (c) Median water content residuals versus water content SD (wt.%) for the T-independent hygrometer. (d) Median water content residuals versus water content SD (wt.%) for the T-dependent hygrometer. (e) Median pressure residuals versus pressure SD (MPa) for the H<sub>2</sub>O-independent barometer. (f) Median pressure residuals versus pressure SD (MPa) for the H<sub>2</sub>O-dependent barometer. (g) Median anorthite content residuals versus anorthite content SD (mol%) for the plagioclase-melt equilibria model.

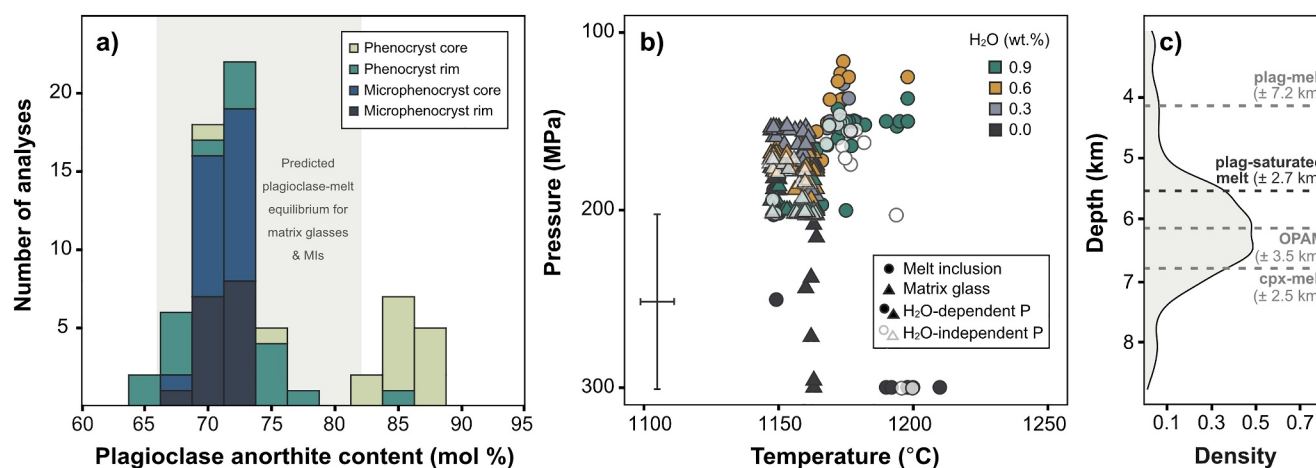


**Figure 9.** (a) Filtered temperature (°C) versus pressure (MPa) predictions of melt inclusions and matrix glasses ( $n = 113$ ) for the 1980 Mount St Helens eruption, estimated using the H<sub>2</sub>O-independent melt thermometer, H<sub>2</sub>O-dependent melt barometer, and H<sub>2</sub>O-independent melt barometer. The histogram on the right displays the saturation pressures of matrix glass ( $n = 29$ ) and melt inclusions ( $n = 45$ ) from Blundy et al. (2010), estimated using the Papale et al. (2006) solubility model. (b) SIMS water contents versus predicted water contents using the T-dependent hygrometer. Color coding reflects SiO<sub>2</sub> content (wt.%) in melt.

941°C; Blundy et al., 2006) calculated using the plagioclase-liquid thermometer of Putirka (2005). Fe-Ti oxide thermometry estimates (816–958°C; Blundy et al., 2008), calculated using the oxide recalculation procedure of Spencer and Lindsley (1981) and the thermometer of Andersen and Lindsley (1988), extend the range to slightly higher temperatures. This slight magma heating may reflect latent heat release due to crystallization or magma recharge (Blundy et al., 2006) and the ability of Fe-Ti oxides to re-equilibrate chemically on short timescales (Venezky & Rutherford, 1999).

We next use the predicted melt temperatures as inputs for the T-dependent hygrometer, producing H<sub>2</sub>O estimates between 2.6 and 6.5 wt.%. We also performed Monte Carlo error propagation using the temperature SD from the thermometer outputs (Figure 9a), and the mean uncertainty for H<sub>2</sub>O predictions across all samples is  $\pm 1.4$  wt.%. A full description of the error propagation method is presented in Text S1 in Supporting Information S1. The majority of melt inclusion H<sub>2</sub>O estimates are broadly similar to the measured analyses by SIMS (Blundy et al., 2006). In contrast, the estimated H<sub>2</sub>O contents for the groundmass and the highly silicic (>75 wt.% SiO<sub>2</sub>) melt inclusions are significantly higher than the measured (Figure 9b) values, reflecting extensive degassing upon eruption and the failure of the melt to evolve chemically in response (Blundy & Cashman, 2005). The comparison could also signify a deficit of highly silicic calibration experiments with low dissolved water concentrations where the H<sub>2</sub>O estimates diverge more profoundly from the 1:1 line. Furthermore, Figure 9b highlights that H<sub>2</sub>O content negatively correlates with SiO<sub>2</sub>, consistent with Blundy and Cashman (2005) suggesting decompression crystallization of the groundmass and plagioclase phenocrysts during ascent.

Finally, using the predicted H<sub>2</sub>O contents as inputs for the H<sub>2</sub>O-dependent barometer, the pressure predictions returned values between 50 and 250 MPa (matrix mean:  $117 \pm 44$  MPa, melt inclusion mean:  $98 \pm 41$  MPa; Figure 9a). We again performed error propagation using the water uncertainty from the hygrometer, resulting in a mean uncertainty of  $\pm 38$  MPa across all samples. The mean uncertainties for both H<sub>2</sub>O and pressure highlight that even with two unknown variables for a system, the accumulated errors are still low enough to obtain informative interpretations; we include the error propagation capability within the provided R scripts (Cutler, 2024). The H<sub>2</sub>O-independent barometer returns similar pressures of 44–225 MPa (matrix mean:  $113 \pm 59$  MPa, melt inclusion mean:  $109 \pm 61$  MPa; Figure 9a). The pressures, particularly from melt inclusions, overlap with saturation pressure values (melt inclusion range: 7–282 MPa; mean: 97 MPa, matrix range: 3.2–20.6 MPa; matrix mean: 8.3 MPa; Figure 9a) from Blundy et al. (2010) estimated using Papale's et al. (2006) H<sub>2</sub>O-CO<sub>2</sub> solubility model. Overall, the main pressure range (44–250 MPa) resulting from both barometers convert to depths of 1.2–6.9 km using a 2700 kg/m<sup>3</sup> average crustal density. Scandone and Malone (1985) estimated a reservoir depth of 7–9 km using net edifice subsidence measured from electronic tiltmeters. An aseismic zone was also mapped at 7 km extending vertically for 6+ km from earthquake hypocenters, and interpreted as a reservoir connected to the surface (Lees, 1992; Scandone & Malone, 1985). Although our mean melt inclusion and matrix glass crystallization depths are shallower than geophysical estimates, the glass compositions likely record crystallization



**Figure 10.** (a) Stacked histogram displaying the composition of plagioclase phenocrysts and microphenocryst crystals from the 2014–2015 Holuhraun eruption (data from Halldórsson et al. (2018)), with the light gray field representing the plagioclase compositions predicted to be in equilibrium with the carrier liquid and inclusions. (b) Filtered temperature (°C) versus pressure (MPa) predictions of melt inclusions and matrix glasses ( $n = 248$ ) for the 2014–2015 Holuhraun eruption, calculated using the H<sub>2</sub>O-independent melt thermometer, H<sub>2</sub>O-dependent melt barometer, and H<sub>2</sub>O-independent melt barometer. Color coding depicts the H<sub>2</sub>O content (wt.%) used as H<sub>2</sub>O-dependent barometer input. (c) Density distribution of dyke seismicity (15 to 30 August 2014;  $n = 273$ ) prior to the eruption; data taken from Ágústsdóttir et al. (2019). Dashed lines represent mean depths estimated from plagioclase-liquid barometry (Geiger et al., 2016) using Equation 25a (Putirka, 2008), plagioclase-saturated melt barometry (mean of both matrix glass and melt inclusion pressures estimated from both H<sub>2</sub>O-dependent and H<sub>2</sub>O-independent melt barometers), OPAM barometry (Hartley et al., 2018), and clinopyroxene-liquid barometry (Neave et al., 2019) using iterative thermobarometric calculations of Equation 1 of Neave and Putirka (2017) and Equation 33 of Putirka (2008).

conditions during pre-eruptive ascent from the top of the storage region, consistent with the H<sub>2</sub>O versus SiO<sub>2</sub> relationship in Figure 9b.

#### 4.2. 2014–2015 Holuhraun Eruption, Bárðarbunga, Iceland

In mid-August 2014, a dyke propagated laterally NE from Bárðarbunga volcano, and by the end of August, the dyke caused a fissure eruption at the Holuhraun lava field (Ágústsdóttir et al., 2016). The Holuhraun magma was a phenocryst poor ( $\leq 5$  vol%), highly vesicular olivine tholeiite (Halldórsson et al. (2018)). Here, we use the basaltic matrix glass and plagioclase-hosted melt inclusion (with post-entrapment crystallization corrections) data ( $n = 251$ ) from Hartley et al. (2018) and Halldórsson et al. (2018). Matrix glass data points with  $< 6$  wt.% MgO were removed, as they represent syn-emplacement crystallization conditions (Halldórsson et al., 2018). We tested the plagioclase-saturation classifier on the matrix glasses ( $n = 175$ ), and 174 compositions were predicted to be plagioclase-saturated, in agreement with the petrography of the samples (plagioclase-olivine-clinopyroxene-Fe-Ti oxides; Halldórsson et al., 2018). Although the one matrix glass composition that failed the classifier test could be, in fact, plagioclase-saturated (i.e., false negative), the main objective of the classifier approach is to eliminate any false positives that may generate inaccurate pressure estimates. We thus removed the single matrix glass composition for subsequent P-T-H<sub>2</sub>O-An estimations.

The modal equilibrium plagioclase compositions predicted for matrix glasses and melt inclusions are An<sub>70</sub> and An<sub>79</sub>, respectively, consistent with the estimated equilibrium plagioclase phenocryst rims and microphenocrysts using the plagioclase-melt equilibria model of Namur et al. (2012) (An<sub>64.5–75</sub>; Halldórsson et al., 2018; Figure 10a). A subset of melt inclusions with higher MgO contents ( $> 8$  wt.%) have higher An<sub>75–82</sub> contents, which likely represent the entrainment of plagioclase phenocrysts from mush horizons (Hartley et al., 2018) now in disequilibrium with the surrounding melt.

Temperature reconstructions for matrix glasses and melt inclusions ( $< 8$  wt.% MgO) with the H<sub>2</sub>O-independent thermometer yield mean temperatures of  $1157 \pm 14^\circ\text{C}$  and  $1176 \pm 13.5^\circ\text{C}$  (Figure 10b), respectively, consistent with clinopyroxene-liquid thermometry ( $1161 \pm 11^\circ\text{C}$ ; Neave et al., 2019) using Equation 33 of Putirka (2008), whereas the primitive melt inclusions (higher MgO) record a higher mean temperature of  $1203 \pm 13^\circ\text{C}$  (Figure 10b). Water contents in matrix glasses and melt inclusions have been measured by FTIR and calculated, accounting for diffusive re-equilibration of melt inclusions, to be in the range of 0.13–0.7 wt.% (Bali et al., 2018; Hartley et al., 2018). If water contents are constrained to a specific range, we can use the H<sub>2</sub>O-



dependent barometer differently by testing various water values as inputs. We use values of 0.0, 0.3, 0.6 and 0.9 wt.% (Figure 10b), and the barometer returns matrix glass pressures of 151–296 MPa (mean:  $185 \pm 94$  MPa) and melt inclusion pressures of 116–300 MPa (mean:  $164 \pm 99$  MPa) for all water contents; varying the water content results in only minor pressure differences ( $\sim 10$ –25 MPa). The H<sub>2</sub>O-independent barometer gives similar matrix glass and melt inclusion pressures ranging between 191 and 202 MPa (mean:  $191 \pm 97$  MPa) and 176–300 MPa (mean:  $176 \pm 91$  MPa), respectively. All mean pressure predictions are in good agreement (Figure 10c) with pressures estimated by clinopyroxene-liquid barometry ( $232 \pm 86$  MPa, Neave et al., 2019; using iterative thermobarometric calculations including Equation 1 of Neave & Putirka, 2017 and Equation 33 of Putirka, 2008), plagioclase-liquid barometry ( $141 \pm 247$  MPa, Geiger et al., 2016; using Equation 25a of Putirka, 2008), and OPAM thermal minima (matrix glass:  $210 \pm 70$  MPa, melt inclusion:  $350 \pm 170$  MPa) with OPAM pressures for primitive melt inclusions returning values of 300–350 MPa (Hartley et al., 2018). Using a crustal density of  $2860 \text{ kg/m}^{-3}$  (Carlson & Herrick, 1990), the ML barometer pressures convert to depths of 3.4–8.8 km. These depths correspond well with the location of earthquake hypocenters (5–7 km; Figure 10c) associated with dyke propagation prior to the eruption (Ágústsdóttir et al., 2019; Sigmundsson et al., 2015).

Overall, the plagioclase-saturated melt models are effective at identifying the last-equilibrated composition of plagioclase crystals with the host melt and characterizing key intensive variables at both Mount St Helens and Bárðarbunga. This is shown by the generally good agreement of predictions with previous petrological estimates using different models (e.g., volatile solubility and mineral  $\pm$  melt thermobarometry) and geophysical data. Comparison of direct H<sub>2</sub>O measurements with hygrometer predictions may also provide insight into which melt inclusions have likely lost water during ascent and their original water contents. The models offer the additional benefit of not requiring saturation of a specific mineral assemblage, which can often restrict the application of many melt-based models (e.g., olivine-plagioclase-augite, OPAM, Yang et al., 1996; Rhyolite-MELTS; Gualda & Ghiorso, 2014).

## 5. Conclusions

We have tested various plagioclase-based hygrothermobarometric models using either plagioclase-melt or melt chemistry and developed an updated plagioclase-melt equilibria model, with all models calibrated using random forest machine learning. Our results show that the melt compositional information holds nearly all the P-T-H<sub>2</sub>O information rather than the plagioclase, resulting in the melt and plagioclase-melt models returning incredibly similar cross-validation RMSE values. Test set RMSEs for the melt + T/H<sub>2</sub>O and melt-only models are 25°C–35°C, 0.65–1.00 wt.%, 74–88 MPa and 5.8 mol% for temperature, water content, pressure and anorthite content, respectively. In general, the models provide enhanced prediction accuracy for P-T-H<sub>2</sub>O and anorthite content values. Furthermore, the T and H<sub>2</sub>O-independent melt hygrothermobarometers allow predictions to be obtained without requiring additional inputs (P/T/H<sub>2</sub>O) that are inherent within all previous plagioclase-based hygrothermobarometer formulations (Masotta & Mollo, 2019; Putirka, 2008; Waters & Lange, 2015), introducing further uncertainties that are often not propagated. For the T and H<sub>2</sub>O-dependent melt hygrothermobarometers, there are dedicated R scripts (Cutler, 2024) to perform error propagation (for either measured H<sub>2</sub>O contents, independent T values, or calculated T/H<sub>2</sub>O estimates from melt-only models) or to generate predictions with T or H<sub>2</sub>O values in a given range.

Application of the melt thermometers and hygrometers is suitable for a wide range of plagioclase-bearing melts across temperatures of 664–1355°C and H<sub>2</sub>O contents  $\leq 11.20$  wt.%; the melt barometer is only appropriate for pressures of  $\leq 500$  MPa. The plagioclase-saturated melt models were applied to melt inclusions and matrix glass from the 1980 Mount St Helens eruption and 2014–2015 Holuhraun eruption, with P-T-H<sub>2</sub>O-An predictions returning consistent constraints comparable to estimates and observations from melt inclusion analyses, geophysical data, and previous hygrothermobarometric and plagioclase-equilibria models. The new set of models enables a quick assessment of plagioclase-melt equilibrium and an insight into the last-equilibrated P-T-H<sub>2</sub>O conditions of plagioclase-bearing magmas in the upper crust.

## Data Availability Statement

All experiments in the calibration datasets are listed in Table S1 in Supporting Information S2 and Table S3 but can also be accessed at <https://doi.org/10.5281/zenodo.10841557> (Cutler, 2024). Figures were made with R

Studio version 4.3.1 (available under the license AGPL version 3 or later: <https://posit.co/downloads/>) and edited in Affinity Designer 2. The R scripts (version 1.0) associated with this manuscript are licensed under MIT and preserved at <https://doi.org/10.5281/zenodo.10841557> (Cutler, 2024). A user-friendly web app of the models can be found under the README section at <https://github.com/kyra-cutler/Plag-saturated-melt-P-T-H2O-An>. Updates to the models will also be available at <https://github.com/kyra-cutler/Plag-saturated-melt-P-T-H2O-An>.

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