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A microkinetic model of temperature dependent silicate dissolution: albite from 100 to 300 °C

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We have used our recently developed microkinetic model for silicate dissolution[1] to fit and understand the molecular scale implications for the high temperature dissolution rate for the aluminosilicate feldspar mineral albite in the range 100-300 °C. We used a statistical calibration by maximum-likelihood estimation with a Gaussian-process likelihood to the experimental dataset [2] as a function of pH at 100, 200, and 300 °C (Figure 1).

We conducted a Sobol' sensitivity analysis and high-dimensional visualization to identify dominant parameter controls and trade-offs. We found that the simultaneous fitting of dissolution rates for three different temperatures required small changes to our original model[1] to reproduce the data.

- The enthalpy barriers had to be decreased to capture the change in dissolution with temperature. Concurrently, the addition of an active site density was necessary to reproduce the absolute dissolution rate. While hinted at this in our original publication, without temperature dependent data to compare to, any active site density was implicitly included in the original enthalpy barriers. This suggests that dissolution occurs on e.g. step sites.
- The fit was better with the assumption that surface pKa shift with temperatures, assumed to follow the temperature dependence for pKw for water, which agrees with experimental observations of how the point of zero charge for minerals shifts with temperature.
- The site dependent barriers were still similar to the original model fits to quartz, amorphous silica, anorthite and amorphous aluminosilicate glass, showing the general applicability of the microkinetic model.

In summary, we were able to fit the high temperature dissolution data within experimental uncertainties by refining our microkinetic model. The non-empirical foundation of the model leads to molecular scale interpretable implications and should allow for more reliable modelling of high temperature dissolution for other silicate materials as well, including how surface pKa shift with temperature.

[1] M.P. Andersson, S.M. Ramsheh, A.M. Schade, J.D. Kubicki, M. Turchi, T.R. Walsh, D. Okhrimenko, M. Solvang, S.L.S. Stipp, *Chem. Geol.* 692 (2025) 122960. https://doi.org/10.1016/J.CHEMGEO.2025.122960.

[2] R. Hellmann, *Geochim. Cosmochim. Acta* 58 (1994) 595–611. https://doi.org/10.1016/0016-7037(94)90491-X.

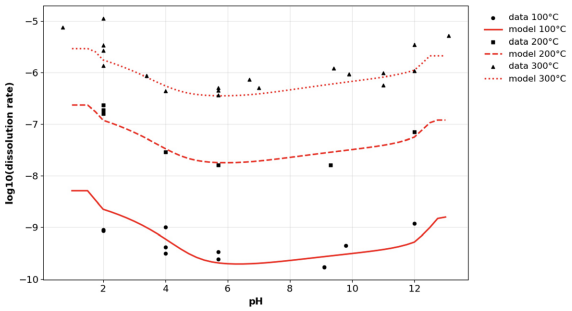

Figure 1. *Albite dissolution rate* $\left(\frac{mol}{m^2 s}\right)$ *versus pH at 100, 200 and 300 °C (symbols: experimental data; lines: calibrated microkinetic model).*