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Towards Optimal P-T Estimates: An Inverse Method for Quantifying P-T Conditions and Uncertainty in Phase Equilibrium Modelling

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Phase equilibrium modelling is reliant on quantitative solution models and thermodynamic databases. However, metamorphic studies often use qualitative to semi-quantitative comparisons between forward-modelled and natural datasets while overlooking or being unable to quantity fundamental sources of uncertainty associated with the input data or the technique. Accurately constraining these uncertainties is essential for extracting reliable insights from petrological studies and interpreting the data within a well-defined range of confidence.

This study presents an inverse method for quantitatively determining the best-fit pressure-temperature (P-T) conditions and associated uncertainties for a given rock system. The technique calculates the difference (misfit) between observed data (e.g., mineral compositions, modal volumes) and forward model predictions across a user-defined P-T grid, identifying the lowest-misfit point as the best-fit solution. Bootstrap resampling (repeatedly sampling the dataset with replacement) quantifies the uncertainty of the inverse solution and evaluates the sensitivity of the inversion to uncertainty in individual input variables. Additionally, three diagnostic metrics—quality of data fit, standard error, and variable sensitivity—are implemented to validate and refine the best-fit solution.

The workflow is applied to a kyanite-zone pelite from the Greater Himalayan Sequence in the Zanskar Himalaya, northwest India. The estimated peak P-T conditions (median: 576°C, interquartile range 573–582°C; 9.5 kbar, interquartile range 9.3–9.8 kbar) align with results from classical thermobarometric methods, including conventional thermometry, multi-equilibrium barometry, and the pseudosection peak assemblage field.

To assess broader trends in P-T uncertainty across sub-solidus metamorphic conditions, the workflow is applied to the worldwide median pelite composition[1]. The results show that P-T uncertainty varies significantly with metamorphic grade. Lower-grade conditions exhibit nearly twice the uncertainty of higher-grade conditions, with uncertainties ranging from 25–30°C and 1.2–1.8 kbar in lower-grade rocks (biotite and garnet zones) compared to 16°C and 0.8 kbar in higher-grade rocks (cordierite/andalusite/staurolite/kyanite and sillimanite zones). A similar trend is observed across facies series, with the highest temperature uncertainty occurring in the lowest-pressure cordierite-andalusite-sillimanite series (29°C) and the lowest temperature uncertainty in the staurolite-kyanite-sillimanite series (16°C). In contrast, pressure uncertainty remains relatively consistent across all facies series, ranging from 0.9 to 1.1 kbar.

[1] Forshaw, J. B., & Pattison, D.R.M. *(2023), Geology* 51, 39–43.