

## **Constraints on non-isothermal diffusion modeling: An experimental analysis and error assessment using halogen diffusion in melts**

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### **ABSTRACT**

Diffusion chronometry on zoned crystals allows constraining duration of magmatic evolution and storage of crystals once temperatures are precisely known. However, non-isothermal diffusion is common in natural samples, and thus timescales may not be determined with confidence while assuming isothermal conditions. The “non-isothermal diffusion incremental step (NIDIS) model” (Petroni et al. 2016) is proposed for such cases for a non-isothermal diffusive analysis. We conducted diffusion experiments with stepwise temperature changes to analyze and test the model, evaluated the associated errors and improved the accuracy by suggesting an alternative algorithm to model diffusion times.

We used Cl and F ( $\leq 0.4$  wt%) as the diffusing elements in nominally anhydrous ( $H_2O \leq 0.3$  wt%) phonolitic melt with composition of Montana Blanca (Tenerife, Spain) in an experimental setup that successively generates multiple diffusive interfaces for different temperatures by adding glass blocks of different Cl and F concentrations. This compound set of two diffusion interfaces represents distinct compositional zones that diffusively interact at different temperatures, which can be taken as an equivalent to non-isothermal diffusion in zoned magmatic crystals. The starting temperature ranged from 975 to 1150 °C, and each set of experiments included a temperature change of 85–150 °C and a total duration of 8–12 h. The experiments were carried out in an internally heated pressure vessel equipped with a rapid quench device at 1 kbar pressure. Cl and F concentration profiles were obtained from the quenched samples by electron microprobe analysis. Although the estimated diffusion times from the NIDIS-model matched well with true experimental values, the errors on estimated timescales, due to errors in curve-fitting and uncertainty in temperature, were  $\pm 10$ –62% ( $1\sigma$ ). The errors are much larger at 61–288% ( $1\sigma$ ) when the uncertainty in diffusivity parameters is included. We discuss the efficiency and limitations of the model, assess the contribution from different sources of error, and their extent of propagation. A simpler alternative algorithm is proposed that reduces errors on the estimates of diffusion time to 10–32% ( $1\sigma$ ) and 60–75% ( $1\sigma$ ), with and without including uncertainty in diffusivity parameters, respectively. Using this new algorithm, we recalculated the individual diffusion times for the clinopyroxene crystals analyzed by Petroni et al. (2016) and obtained a significantly reduced error of 26–40% compared to the original error of 61–100%. We also analyzed a sanidine megacryst from Taapaca volcano (N. Chile) as a test case for non-isothermal modeling and obtained diffusion times of 1.5–9.4 ky, which is significantly different from isothermal analyses including a previous study on similar sample. In this analysis, the error estimated by our new method is reduced by 63–70%.

**Keywords:** Non-isothermal diffusion, diffusion experiment, error assessment, electron microprobe, halogen diffusion