

DIPRA: A user-friendly program to model multi-element diffusion in olivine with applications to timescales of magmatic processes

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(Auxiliary Material 2: Uncertainties in the diffusion times)

One difficulty that potential users of DIPRA find is to know the uncertainty of the diffusion time that best fit the natural data. We have implemented in our code a detailed error analysis of the best time, including those related to the data and related to the uncertainties of the temperature. Errors associated to the cell size Δx and to the interpolation process are not considered. But in general the results will be more accurate for finer meshes as in any other numerical scheme and can be minimized as to be negligible. The calculation process of the uncertainty is as follows:

- a. Users choose the size of the error bars of the experimental concentrations according to the natural data noise and instrumentation.
- b. While DIPRA determines the best fit curve by selecting the minimum *rms*, the number of theoretical concentrations which are not inside the error bars of the data is computed. We call *discrepancy* of the model to the ratio between this number and the total number of data (N ; see Figure 3 of the main text). In an ideal case the discrepancy should be zero for appropriate boundary and initial conditions. For cases

where the discrepancy is large it might be inferred that processes besides diffusion may have occurred (e.g., a large component of growth zoning).

- c. The program calculates the number of curves above (m) and below (n) the best fit that have the same discrepancy as the best fit. The possible solutions are all the curves for which the discrepancy is the smallest one. Therefore, the actual diffusion time must be in the interval:

$$\{t - (m + 1)\Delta t, t + (n + 1)\Delta t\} \quad (1)$$

- d. On the other hand, most geothermometers may have uncertainties of $\sigma(T) = \pm 30^\circ\text{C}$ (Costa *et al*, 2008; see references in main text). This leads to an uncertainty on the diffusivity and therefore on time. Time and diffusion coefficients are scaled by $t \propto 1/D$ while $D \propto \exp(\tau_i/T)$, being τ_i the factors that appear in the exponentials of the Table 1 except the temperature (i : Fo, Mn, Ni, and Ca). For the case of Ca, we consider that τ_{Ca} is just the average of the exponential terms of the three crystallographic axes. Therefore, for the best fit:

$$t \propto \exp(-\tau_i/T) \quad (2)$$

However, the actual diffusion time may vary between $t_- < t < t_+$, being:

$$t_- \propto \exp(-\tau_i/[T + \sigma(T)]) \quad (3)$$

$$t_+ \propto \exp(-\tau_i/[T - \sigma(T)]) \quad (4)$$

By combining the equations 2-4 we can calculate t_- and t_+ as a function of the best time t :

$$t_- = t \cdot \exp \left[\tau_i \left(\frac{1}{T} - \frac{1}{T+\sigma(T)} \right) \right] \quad t_+ = t \cdot \exp \left[\tau_i \left(\frac{1}{T} - \frac{1}{T-\sigma(T)} \right) \right] \quad (5)$$

In summary, DIPRA calculates the following uncertainty for the diffusion time by considering the conditions 1 and 5:

$$\sigma(t) = \left\{ \begin{array}{l} + \left\{ (n+1)\Delta t + t \left[\exp \left[\tau_i \left(\frac{1}{T} - \frac{1}{T-\sigma(T)} \right) \right] - 1 \right] \right\} \\ - \left\{ (m+1)\Delta t + t \left[1 - \exp \left[\tau_i \left(\frac{1}{T} - \frac{1}{T+\sigma(T)} \right) \right] \right] \right\} \end{array} \right\} \quad (6)$$

This error depends on the diffusion time, on the time step, and on the temperature and its uncertainty. It is higher for larger diffusion times and lower for larger temperatures. It is not symmetrical in general. The second term becomes dominant for larger uncertainties in the temperature and lower uncertainties in the concentrations measured in the lab.