

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 1: Discretization of the diffusion equation in olivine)

A numerical method is needed to solve the diffusion equation because analytical solution exists only for very simple situations. Here we choose the method of finite differences explicit in time because it is computationally fast for our purposes and implicit schemes are rather more complicated when the diffusivity is not constant. The scheme that we use is forward difference in time and second-order accurate central difference for the space derivative. Diffusion equation is replaced by an algebraic equation where the variables are the concentrations at some discrete points:

$$\frac{\partial \theta_i^{k,j}}{\partial t} = \frac{dD_i}{d\theta_{Fo}} \bigg|_{\theta_{Fo}^{k,j}} \frac{\partial \theta_{Fo}^{k,j}}{\partial x} \frac{\partial \theta_i^{k,j}}{\partial x} + D_i \bigg|_{\theta_{Fo}^{k,j}} \frac{\partial^2 \theta_i^{k,j}}{\partial x^2} \quad (1)$$

i represents Fo, Mn, Ni, or Ca; k and j refer to the spatial and time steps indexes, respectively. By using the Taylor expansion up to first order we can replace the first derivatives by finite increments:

$$\theta_i^{k+1,j} \approx \theta_i^{k,j} + \Delta x \frac{\partial \theta_i^{k,j}}{\partial x} \rightarrow \frac{\partial \theta_i^{k,j}}{\partial x} \approx \frac{\theta_i^{k+1,j} - \theta_i^{k,j}}{\Delta x} \quad (2)$$

$$\theta_i^{k,j+1} \approx \theta_i^{k,j} + \Delta t \frac{\partial \theta_i^{k,j}}{\partial t} \rightarrow \frac{\partial \theta_i^{k,j}}{\partial t} \approx \frac{\theta_i^{k,j+1} - \theta_i^{k,j}}{\Delta t} \quad (3)$$

By expanding up to second order we obtain the approximation for the laplacian term:

$$\theta_i^{k+1,j} \approx \theta_i^{k,j} + \Delta x \frac{\partial \theta_i^{k,j}}{\partial x} + \frac{1}{2} \Delta x^2 \frac{\partial^2 \theta_i^{k,j}}{\partial x^2} \quad (4)$$

$$\theta_i^{k-1,j} \approx \theta_i^{k,j} - \Delta x \frac{\partial \theta_i^{k,j}}{\partial x} + \frac{1}{2} \Delta x^2 \frac{\partial^2 \theta_i^{k,j}}{\partial x^2} \quad (5)$$

By adding the last two equations we obtain:

$$\theta_i^{k+1,j} + \theta_i^{k-1,j} \approx 2\theta_i^{k,j} + \Delta x^2 \frac{\partial^2 \theta_i^{k,j}}{\partial x^2} \rightarrow \frac{\partial^2 \theta_i^{k,j}}{\partial x^2} \approx \frac{\theta_i^{k+1,j} - 2\theta_i^{k,j} + \theta_i^{k-1,j}}{\Delta x^2} \quad (6)$$

If we replace equations (2), (3), and (6) in the diffusion equation (1) we obtain:

$$\frac{\theta_i^{k,j+1} - \theta_i^{k,j}}{\Delta t} = \frac{dD_i}{d\theta_{Fo}} \bigg|_{\theta_{Fo}^{k,j}} \frac{\theta_{Fo}^{k+1,j} - \theta_{Fo}^{k,j}}{\Delta x} \frac{\theta_i^{k+1,j} - \theta_i^{k,j}}{\Delta x} + D_i \bigg|_{\theta_{Fo}^{k,j}} \frac{\theta_i^{k+1,j} - 2\theta_i^{k,j} + \theta_i^{k-1,j}}{\Delta x^2} \quad (7)$$

The diffusivity and its derivative are not discretized because there are empirical relationships which link the diffusivity with the concentration of Fo (Table 1 of the main text). We can finally write the concentration in one forward time step.

$$\theta_i^{k,j+1} = \theta_i^{k,j} + \frac{\Delta t}{(\Delta x)^2} \left\{ (\theta_i^{k+1,j} - \theta_i^{k,j}) (\chi_{Fo}^{k+1,j} - \chi_{Fo}^{k,j}) \frac{dD_i}{d\chi_{Fo}} \bigg|_{\chi_{Fo}^{k,j}} + (\theta_i^{k+1,j} - 2\theta_i^{k,j} + \theta_i^{k-1,j}) D_i \bigg|_{\chi_{Fo}^{k,j}} \right\} \quad (8)$$

Δx is the size of the one-dimensional cell; and Δt is the size of the time step. In the above equations we have considered that the diffusivities are expressed as functions of the concentration of Fo in units of mole fraction. The concentration units of Mn, Ni, and Ca can be given according to the user choice.