Diffusion in minerals and melts: a primer for graduate and senior undergraduate students

Cliff S.J. Shaw

Department of Earth Sciences, University of New Brunswick, P.O. Box 4400, Fredericton, New Brunswick E3B 5A3, Canada

<cshaw@unb.ca>

Although chemical diffusion is ubiquitous in high temperature geological systems, it is usually not given much time in undergraduate courses since students recoil at the complex mathematical procedures that are needed to analyze diffusion data. Although the equations are sometimes long and have unfamiliar terms, they can be solved quite easily using the SOLVER function in MICROSOFT EXCEL.

Any process in which a chemical potential gradient is generated will result in diffusive mass transfer of chemical components which in turn will result in development of a diffusion profile whose length will vary depending on the time and diffusion coefficient. The chemical diffusion process is divided into three groups, each of which has its own set of solutions to the diffusion equations: (1) binary diffusion e.g. Fe-Mg interdiffusion in between two olivine crystals of different composition; (2) ternary diffusion between simple three component melts such as those used in analogue models of magma behaviour e.g. the $CaOAl_2O_3$-SiO_2 system; and (3) multicomponent diffusion in natural systems with more than three chemical components.

If we know the diffusion coefficient we can determine the duration of the diffusion process, or, if we control the duration of the diffusion process we can extract the diffusion coefficients. In all cases a detailed chemical profile across the sample starting at the source of the diffusing element and ending in the region unaffected by diffusion is required. With this information in hand we can set up simple models in MICROSOFT EXCEL in which we iteratively change one or more parameters in order to minimize the sum of the squares of the difference between the measured and modelled compositions.

Regardless of the type of diffusion profile being modelled, we need to use a solution to a partial differential equation. Fortunately, there are "cookbooks" available that give every imaginable solution to the diffusion equation. The three scenarios above all use a similar formulation that involves examining the difference between the initial and final composition of the profile points for a fixed diffusion rate over a fixed time. All three use the error function, which is the source of most of the trepidation that students experience when confronted with this kind of problem. A step by step walk-through is provided for the three types of diffusion problem described above so that with practice and some knowledge of EXCEL, students will be able to work with simple diffusion models.

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