EOS 240: Lab Assignment 3

Trace element partitioning during crystallization

Due: 2:30 pm February 08, 2024 (Th section)
Due: 1:30 pm February 09, 2024 (F section)

You have one week to complete this assignment. You should submit your response to the course Brightspace page as a single PDF file. **Additionally, we ask that you upload a copy of the scripts, code, or spreadsheets you used to complete the assignment. These documents will help us track down mistakes.** Responses to questions should be typed, using complete sentences and standard grammar. If you choose to support your answers with hand-drawn illustrations or hand-written calculations, you should scan or photograph the written work and integrate it into your PDF file as a figure. Double check that your image resolution is high enough to read. A google search of 'PDF combiner' will return a number of webpages that allow you to upload individual images and combine them into a single .pdf file (example: combinepdf.com). There are also a number of good apps for mobile phones. If you write your response in a word processor, please export to .PDF before submitting your response.

You are not excluded from working with others (pairs are recommended), but each person will submit their own copy of the assignment. In your submission, include the names of anyone you worked with on the assignment.

To answer the questions, you can perform calculations and make figures using Excel (an open source alternative: www.libreoffice.com), or with a program or programming language of choice.

Name : _____

Page:	3	4	5	**Total:**
Marks:	8	4	5	17
Score:				

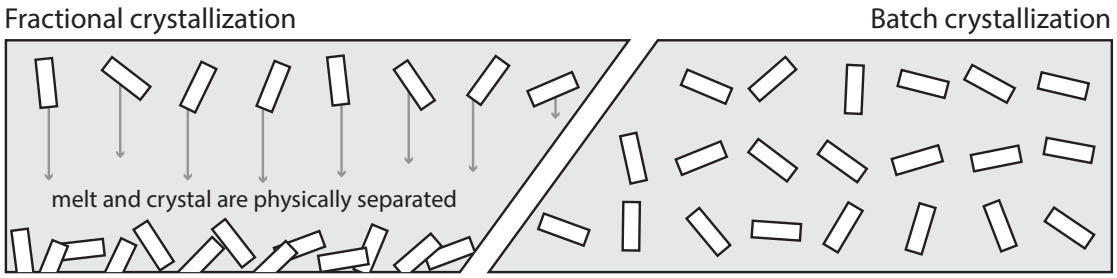

Figure 1: In this assignment, you will explore how two different models of crystallization provide distinct predictions about the behavior of trace elements in the minerals precipitating from a melt. Fractional crystallization describes an open system process where the crystallizing mass is removed or physically separated from the melt. On the other hand, batch crystallization describes a process where the melt and crystals remain in equilibrium.

Introduction

In this lab, you will compare **Ni** concentrations in olivines to modeled predictions of **Ni** concentrations during *batch* and *fractional* crystallization. You will find the partition coefficients, D, that best fit each crystallization model, and you will compare those results to experimentally determined partitioning for **Ni** to argue for which crystallization model more accurately describes the magmatic system that these olivine samples formed in. Recall:

The **partition coefficient**, D, describes the ratio of concentrations for an element between a mineral and a melt at equilibrium:

$$D = \frac{C_S}{C_L}$$

Batch crystallization describes a scenario where some fraction of a magmatic system crystallizes and remains in equilbrium with the liquid.

$$\frac{C_S}{C_0} = \frac{D}{F + D(1-F)}$$

Fractional crystallization describes the continuous removal of mineral percipitates from a melt:

$$\frac{C_S}{C_0} = D(F)^{D-1}$$

C is the concentration of a trace element. Subscript L represents the melt phase. Subscript S represents the solid phase. C_0 means at the initial conditions when melt is 100% of the system. D is the partition coefficient, and F is the melt fraction (where 1 is 100% melt).

Question 1 (17)

Nickel contents of basaltic olivines

(a) (2 points) *olivines.txt* contains the chemical composition of 588 olivine mineral separates from basalt. The units are in mass fraction (wt %). These olivines have crystallized out of a basaltic melt, and the major and trace element chemistry of the olivines can tell us about that crystallization process. Make a figure showing the how **Mg**, **Fe**, and **Ni** vary in these olivines. Geochemists use a quantity known as the **Mg#** to describe the **Mg** and **Fe** contents of mafic and ultramafic rocks and minerals. The **Mg#** is defined as:

$$\text{Mg\#} = 100 \times \frac{\text{Mg}}{\text{Mg} + \text{Fe}^{2+}}$$

where **Mg** and $\mathbf{Fe}^{2+}$ are in moles. Your X-axis should be **Mg#** and your Y-Axis should be **Ni** concentration in *parts per million* (ppm; μg per g^{-1}). Label this figure as Figure 1.

(b) (1 point) You have used phase diagrams of olivine in the past to determine that high **Mg#** olivines represent the earliest crystallization of cooling basaltic melt. As more olivine crystallizes, the **Mg#** of the olivine decreases. Given this relationship to crystallization, is **Ni** *compatible* ($D > 1$) or *incompatible* ($D < 1$) in olivine at the range of pressures, temperatures and melt compositions represented by this dataset?

(c) (2 points) You will now use models to predict how the **Ni** content of our olivines will evolve during crystallization. You will use these predictions to determine the most representative partition coefficient, D, for Ni in olivine. For the following, assume that in all cases the very first olivine to precipitate out of our melt has a composition of:

Mg#	92
Ni (ppm)	3500

Mark this spot on your *Figure 1* (it should be near the upper right corner of your data cloud). If this marked composition is the first olivine to precipitate from your melt, what is the starting concentration of **Ni** in your system? Your response should be a function of D, the partition coefficient. *Hint: it is fair to assume F, the fraction of melt, is 1 at this point which means the* $C_L = C_0$.

(d) (3 points) Make a new figure (Figure 2) showing how the **Ni** concentration in olivine will change as olivine crystallizes from your initial melt. Show the predictions for both *batch crystallization* and *fractional crystallization*. For this figure, assume that the partition coefficient, D, is 10. Your X-axis should be **F**, the fraction of melt, and your Y-Axis should be **Ni** concentration in *parts per million* (ppm; μg per g^{-1}). (It is convention and recommended to plot data as points and models as lines.)

(e) (2 points) The **Mg#** of olivine tracks the crystallization process (it tracks the decrease in the melt fraction F). You are going to assume that **Mg#** changes linearly as F decreases from our initial conditions (part c) where $F = 1$ to an **Mg#** of 75 where $F = 0.875$:

	lower end member (lo)	upper end member (hi)
Mg#	75	92
F (ppm)	0.875	1

You can use a *linear interpolation* between the end members above to determine an unknown **Mg#** for a known F (subscript *lo* refers to the lower end member and subscript *hi* refers to the upper end member in the table above):

$$[\text{unknown Mg\#}] = \text{Mg\#}_{\text{lo}} + ([\text{known F}] - \text{F}_{\text{lo}}) * \frac{\text{Mg\#}_{\text{hi}} - \text{Mg\#}_{\text{lo}}}{\text{F}_{\text{hi}} - \text{F}_{\text{lo}}}$$

This formula can also be understood as a weighted average. The weights are inversely related to the distance from the end points to the unknown point; the closer point has more influence than the farther point. Use this formula to convert F, the melt fractions from part d into estimated **Mg#**s for both *batch crystallization* and *fractional crystallization*. Use these estimated **Mg#**s to add the calculations from part d to Figure 1. Label each model line.

(f) (2 points) You are now able to change the partition coefficient, D, in your crystallization models to compare, visually, how well the model fits the data. Presumably, the best fit of the more accurate model should correspond to the real partition coefficient for Ni in the magmatic systems sampled by these olivines. Using just your eyes, adjust your partition coefficients to find a good fit for each model. List each coefficient:

Model	D
batch crystallization	???
fractional crystallization	???

(g) (5 points) It can be challenging to compare models and noisy data by eye. For this part, you will calculate the the misfit between your models and the data. First, you will need to determine the melt fraction F for each data point using the observed **Mg#**. This calculation is identical to part e, except that we are going in the opposite direction (from a known **Mg#** to an unknown F):

$$[\text{unknown F}] = \text{F}_{\text{lo}} + ([\text{known Mg\#}] - \text{Mg\#}_{\text{lo}}) * \frac{\text{F}_{\text{hi}} - \text{F}_{\text{lo}}}{\text{Mg\#}_{\text{hi}} - \text{Mg\#}_{\text{lo}}}$$

Next, using each sample's estimated F you can calculate the *expected* **Ni** content directly with the *batch crystallization* and *fractional crystallization* equations for a partition coefficient, D, of your choosing. Now for each sample and model, you have a pair of *expected* **Ni**, which we will call **E**, and *observed* **Ni**, which we will call **O**. The *mean squared error* is a statistic that captures how close the dataset is to our model line:

$$mse = \frac{1}{n}\sum_{i=1}^{n}(O - E)^2$$

Calculate the mean squared error of each crystallization model for partition coefficients ranging from $D = 10$ to $D = 30$ in increments of 1 (in other words D =10,11,12,...,29,30):

D	Fractional mse	Batch mse
10	???	???
...	???	???
30	???	???

Laboratory experiments and field data suggest that the partition coefficient of **Ni** in olivine is close to 15 for basaltic melts at the temperatures and pressures covered by these samples. Using this partitioning information and the mean squared errors calculated above, which crystallization model do you believe is more accurate, *batch* or *fractional*? Support your answer with a figure (Figure 3) that shows the misfits between your data and models. Your X-axis should be the partition coefficients used in each experiment, and the Y-axis should be the *mean squared error. A log scale for the Y-axis can be helpful.*