

# Olive 1.1 a simple calculator of fractional crystallization

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## 1 Introduction

This is a little tutorial for Olive 2.0, a calculator for fractional crystallization. Unlike MELTS, Olive does not have a thermodynamic model under the hood so it does not calculate *what phases* are crystallising from a given melt at a given pressure, temperature and oxygen fugacity. Rather, Olive 2.0 calculates the changes in a melt composition given that the fractionated (or added) minerals and their (weight) proportions are prior known.

## 2 Getting started

Let's say you have a basaltic melt and you would like to estimate how such composition would change if olivine, plagioclase and clinopyroxene are fractionating. After launching the tool you will be prompted with the window shown in Figure 1. Enter in the first box the *total amount in grams of melt* and the chemical analysis *in weight percent* below. The total amount of melt is indeed an essential parameter in the calculation, but it is an unknown in most systems<sup>1</sup>. As we shall show below, it is really not an important value if you make the assumption that the melt is homogeneous.

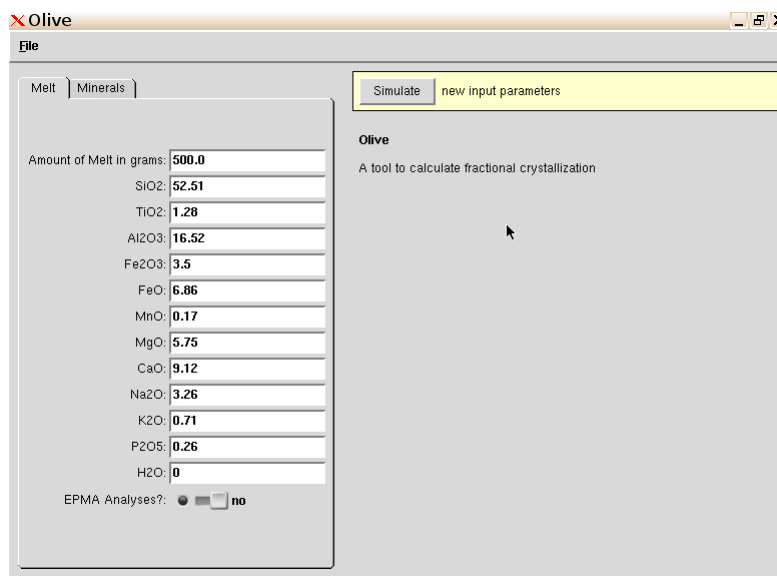


Figure 1: Input screen for the melt composition in weight percent. First value is the absolute amount of melt in grams.

Next, click on the tab for “Minerals” (Forget the “EPMA Analysis” option for now) in which you will be prompted to enter the proportion *in weight* of the different minerals you might want to extract from your melt

<sup>1</sup>unless you are performing some experimental petrology with known amounts!

(Figure 2). The first box is for the total amount *in grams* of extract you might want to use, the next box is the number of steps you want when extracting the solids from the melt. As I said before for the melt, it really doesn't matter the actual absolute values if both the melt and the extract are homogeneous; the only important constraint you really have to know *is the proportion between melt and extract*.

Let's assume you want to fractionate 10% of the melt as solids. Simply fill the amount of total melt with 100 grams and the amount of the extract with 10 grams. In the example, I am using 500 grams of melt and 50 grams of extract, which will produce the same results in wt%, albeit the absolute amounts will be different. Obviously you might use decimal places in both the amount of melt and extract to obtain decimal proportions.

The following box is the number of (equal) steps you want for the extract to be removed or added. This value is an integer that can be positive or negative (zero is also an option but it really doesn't make sense!). If you put a positive value, the extract will be fractionated in that number of steps to finally complete the total mass filled in the box above. A negative value *will add such extract until the total mass desired*. For example 50 grams of minerals in 10 steps will calculate the changes in the melt subtracting 5 grams of minerals (or 1% of the total assuming is 500 grams) in each step, while -10 steps would add 5 grams of minerals in each iteration until 50 grams of minerals are added into the melt.

Let's say you want to extract 40% of olivine, 30% of plagioclase and 30% of clinopyroxene from the melt. Normally, the proportions between melt and crystals are estimated from a thin section as an area percentage as a proxy of the volume% of the different mineral phases, but in general ferromagnesian minerals have densities around  $3 - 3.5 \left[ \frac{gr}{cc} \right]$  while plagioclase is around  $\sim 2.7 \left[ \frac{gr}{cc} \right]$  so the volumetric estimation is a reasonable estimation of the mineral proportion in weight. Beware if your sample contains lots of magnetite ( $\rho \sim 5 \left[ \frac{gr}{cc} \right]$ ) or your olivine is Fayalite ( $\rho \sim 4.4 \left[ \frac{gr}{cc} \right]$ ). If that is the case, you will need to adjust the mineral proportion accordingly.

Next, we need to estimate the actual mineral formula of the mineral phases, since Olive 2.0 input is given in terms of *the proportion of the end members*. An educated guess of that composition can replace any microprobe analysis! In the example I will assume olivine  $Fo_{70}$  and plagioclase  $An_{60}$ . For the pyroxene, Olive expects the composition in terms of three end-members: Wollastonite, Enstatite and Ferrosilite; for the example I will consider that the pyroxene is Diopside, i.e. 50% Wollastonite and 50% of Enstatite.

Because 70% of the olivine is Forsterite, 30% will be Fayalite. With a simple proportion you can easily find that, out of the 40% of olivine 28% is Forsterite and 12% is Fayalite; along the same lines 18% is Anorthite while 12% is Albite. The clinopyroxene is a piece of cake, 50% of 30 is 15.

### 3 EPMA Analyses option

As you might have noticed, below the boxes to Input the melt composition, there is a button to select "EPMA Analyses" (yes/no), which by default is set to "no", to perform the calculation with end members of the fractionated added mineral phases. If you select "yes", then the second tab "Minerals" will change to "Analyses" intended for custom analyses of the mineral phases, likely performed by EPMA. Moving to the tab will show a window for enter up to five custom mineral phases (Figure 3). The input for each mineral phase have 13 number fields separated by spaces, the first value, the weight fraction, followed by  $SiO_2$ ,  $TiO_2$ ,  $Al_2O_3$ ,  $Fe_2O_3$ ,  $FeO$ ,  $MnO$ ,  $MgO$ ,  $CaO$ ,  $Na_2O$ ,  $K_2O$ ,  $P_2O_5$ ,  $H_2O$  in wt%. It doesn't matter if the analysis doesn't close to 100% or the sum of the fractions doesn't close to 100 (or "1"), these values will be normalized for the calculation. If you enter less than 13 values, Olive 2.0 will complain and won't perform the calculation; if you enter more ... the calculation will be performed ignoring the value 14 and beyond.

### 4 Output

No matter what calculation you have selected, clicking in the "Simulate" button at the upper right side will perform the calculation, and will report the results in the output window (Figure 4). The first row will contain the initial composition and its total amount in grams, while the following rows will show how the composition of the melt changes in each iteration, as well as the decrease/increase of the total mass. Below these rows, Olive 2.0 will report the total composition of the extract and the total grams subtracted or added to the original melt.

Clicking on the green arrow will display the download window (Figure 5) that can be then imported to the local machine as a text file that can be easily opened in a spreadsheet application.

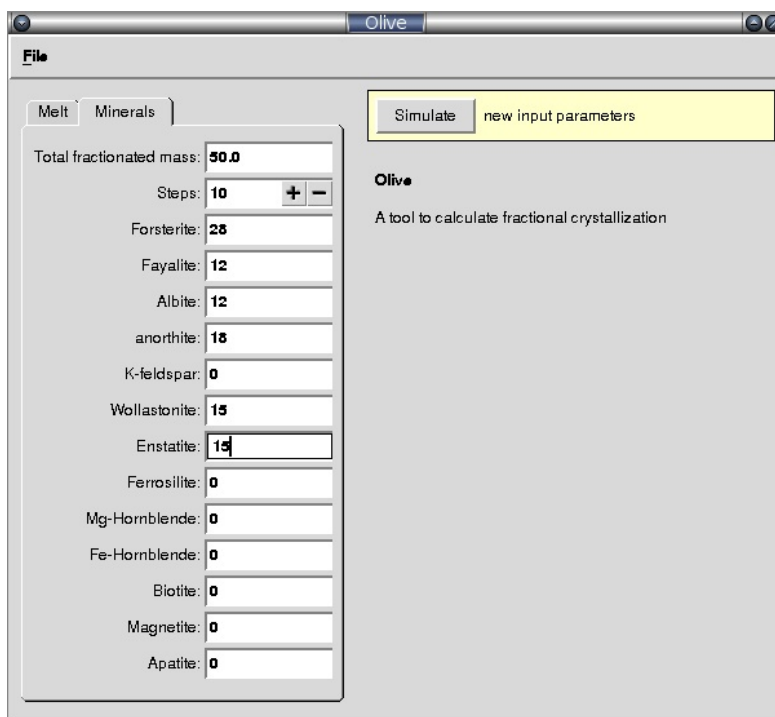


Figure 2: Input screen for the mineral composition in weight percent. First value is the total amount in grams of the mineral phases and second value the number of steps for such extraction.

If there is not enough of a particular element that it is part of the mineral composition of a phase for the first option or for the mineral assemblage for the second, then that phase/assemblage will cease to crystallise. Typically, lack of  $H_2O$  will inhibit crystallization of Hornblende or Biotite in the first option, or a whole assemblage in the second. If that is the case, the output will inform the user below the composition of the solids that a given phase or the whole assemblage didn't crystallise at some step during the calculation.

## 5 Some final remarks

- Olive 2.0 will recalculate your analysis to 100 wt% and the proportion of minerals (end members or EPMA analyses) to 100%, so if you don't want surprises enter in the input boxes already normalised values.
- As I said before, this is just a calculation with no thermodynamic model behind; if you want to test whether these results are realistic, you should use a thermodynamic model such as MELTS.
- Remember if an element is completely used up, then the phase that uses such element won't crystallise; you will be informed of this in the output, but also the amount of extracted solids won't be the total amount of solids entered in the first box. Phases are extracted roughly following the Bowen's series, i.e., more or less how they are sorted in the input window. *Phases are subtracted as end-members; that means that Forsterite is taken independent of Fayalite.* In other words if you lack iron then still olive will subtract Forsterite from the system if it has been selected. I believe this behaviour is more realistic than subtract the solid solution, reflecting the crystallisation phenomenon at a molecular scale. In any case, set up the ratio melt/solid carefully to avoid erratic behaviour. If you have selected to enter analyses, then Olive will calculate the composition of the whole assemblage and will subtract it *as a whole* from the melt.
- Olive 2.0 can be useful to estimate the composition of your groundmass! simply set up the minerals you want to extract, set the steps to one and press "Simulate".

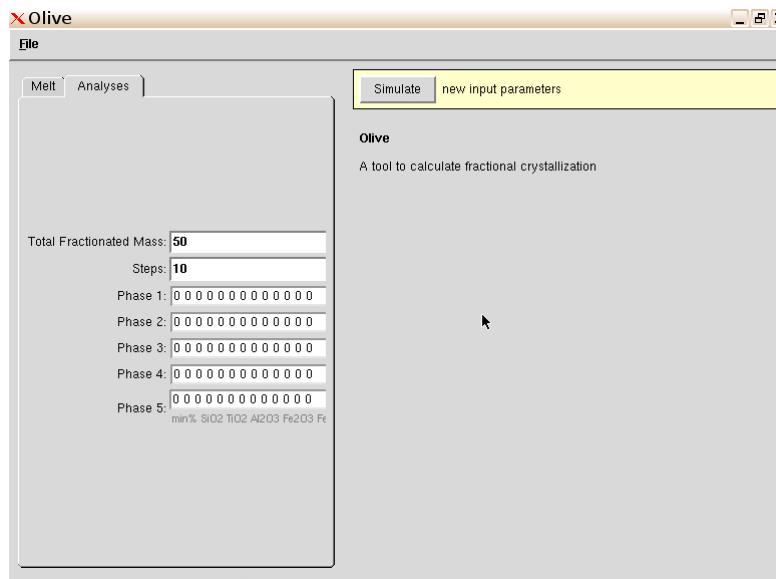


Figure 3: Olive 2.0 ready for input of mineral analyses in wt%

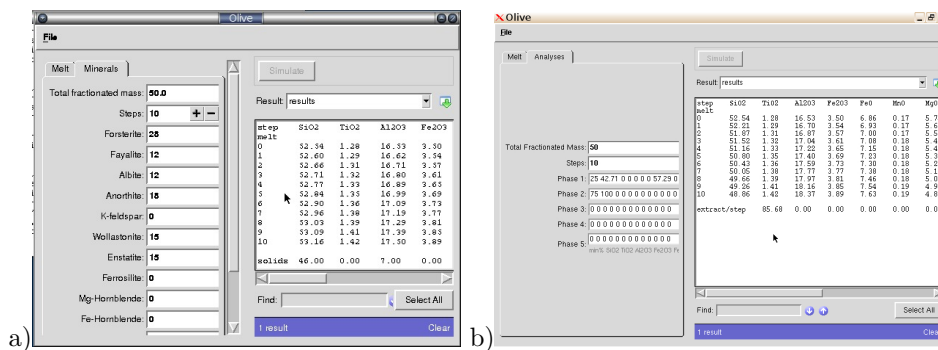


Figure 4: Output window a) option “Minerals”; b) option “EPMA Analyses”, note the right-upper icon with the green arrow to download your results.

- Another possible cool application is magma mixing; enter magma “A” in the first tab, select “EPMA analyses” and enter the composition of magma B in the second tab. Select option -1 for steps and press “Simulate”. Obviously, you can also add magma “B” in steps to simulate a mixing line in a variation diagram.
- You might want to perform a more complex calculation first extracting olivine and then, after few iterations, olivine and plagioclase<sup>2</sup>. Simply run the calculator with olivine and then input the output of that calculation as a new melt with the new desired mineral setting.

<sup>2</sup>... or one phase and then two phases from EPMA analyses!

step	SiO2	TiO2	Al2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	H2O	mass
melt													
0	52.54	1.28	16.53	3.50	6.86	0.17	5.75	9.13	3.26	0.71	0.26	0.00	500.00
1	52.60	1.29	16.62	3.54	6.85	0.17	5.59	9.08	3.28	0.72	0.26	0.00	495.00
2	52.66	1.31	16.71	3.57	6.83	0.17	5.42	9.04	3.30	0.72	0.27	0.00	490.00
3	52.71	1.32	16.80	3.61	6.81	0.18	5.25	9.00	3.32	0.73	0.27	0.00	485.00
4	52.77	1.33	16.89	3.65	6.80	0.18	5.07	8.95	3.34	0.74	0.27	0.00	480.00
5	52.84	1.35	16.99	3.69	6.78	0.18	4.89	8.91	3.36	0.75	0.27	0.00	475.00
6	52.90	1.36	17.09	3.73	6.76	0.18	4.71	8.86	3.38	0.76	0.28	0.00	470.00
7	52.96	1.38	17.19	3.77	6.74	0.18	4.53	8.81	3.40	0.76	0.28	0.00	465.00
8	53.03	1.39	17.29	3.81	6.73	0.18	4.34	8.76	3.42	0.77	0.28	0.00	460.00
9	53.09	1.41	17.39	3.85	6.71	0.19	4.14	8.71	3.44	0.78	0.29	0.00	455.00
10	53.16	1.42	17.50	3.89	6.69	0.19	3.94	8.66	3.47	0.79	0.29	0.00	450.00
solids	46.00	0.00	7.00	0.00	8.00	0.00	22.00	13.00	1.00	0.00	0.00	0.00	50.00

Figure 5: Download window, clicking on the “Save As” message will download your results as a text file you can import to your favourite spreadsheet software ... Libre Office in my case.