PETROGEN ***(a geophysically constrained plagioclase-spinel-garnet mantle melting model)***

Petrogen runs in MATLAB (for now). In theory Petrogen is a single .m function (**PETROGEN2020.m**) with a few other *local functions*. However, given the complexity and variability in mantle melting, and the fact that we want to run more than one melting model at a time, dealing with data management of the results can become a huge mess so we have written a master program **AAA_Master_MeltPlot_Petrogen.m** that walks you through running Petrogen and extracting useful data and plots.

Start off by running **AAA_Master_MeltPlot_Petrogen.m** in the MATLAB command window or by pressing the green "Run" button in the MATLAB editor. You will be given 6 choices of how to proceed:

```
Do you want to:
[1] Run new Petrogen models
[2] Extract submodels for plotting and saving
[3] Plot (3a) or replot (3b) submodel results
[4] Save results to a spreadsheet
[5] Remake paper figures
[6] Import new trace element fractional crystallization Ds?
```

The first four options comprise the bulk of Petrogen, when you wish to run new melting models and make new plots.

You can bypass running Steps 1 and 2 to directly remake some selected paper figures by choosing command [5]. Options [3] and [5] are nearly identical and load data saved previously by running Steps [1] and [2]. In fact, the paper figures available in [5] can can also be made by running [3]– the difference is that selecting [5] requires no other action on your part because it has preserved (preloaded) the conditions needed to make those figures. (But, be warned that you might accidently save over these conditions and change something if you accidently save different Step1 and Step2 files with the same filenames.) You may want to do the same with your new figures!

In some cases, such as Figures 7 and 8, Step [5] runs the exact same scripts as made possible in Step [3] but then modifies figures axis afterwards. In other cases (Figures 5 and 6), Step [3] will only create a one-panel figure.

When you want to run new iterations of Petrogen, you will need to run Steps 1–4. We have tried to make this as painless as possible, but it does require some effort. The easiest way to learn is by running an example Starting at Step 1 and getting through Step 4. You will have to edit some m-files and some Excel spreadsheets along the way. You can navigate to them yourself, or you can start running **AAA_Master_MeltPlot_Petrogen.m**, which should open the files you may need to edit.

EXAMPLE 1: Isobaric batch melting of West Kettle River peridotite from 10–50 kbars for comparison to Walter (1998).

Step 1 Modeling Melts: Run **AAA_Master_MeltPlot_Petrogen.m** , select option [1]. The program will spit out the current melting conditions (i.e., which melting models to run). Enter '**N**'. The program will then open the .m in-file (default file is **AAA_Step1_INFILE.m**) as well as the spreadsheet AAA_PETROGEN_SourcesAndDs.xlsx. Look at the in-file. The requirements and units are listed at the top of the file. We are doing isobaric melting, so need the isobaric batch melting parameters. Now find the code needed for this example (hint: search for "Example 1" in the file) and make sure it is uncommented:

```
worksheetName2Save='Step1_Brownetal2020_Isobaric_KLB';
IsobaricOrPolybaric = 'Isobaric';
forceSpPlag = 'force Sp-Plag Boundary';
Porosity_vary = [1];
PIsobaric_vary =  [10 15 30 40 45 50];
BulkCompositions_vary = [7];
dFdPwaterchange_vary=[10];
initialwatercontent_vary = [0];
MaxF=0.3;
```

These conditions describe 6 models all run with the same porosity (100%) under anhydrous melting conditions using the same single major element bulk composition (#7, WKR as defined in AAA_PETROGEN_SourcesAndDs.xlsx).

Now make sure all other Step1 melting conditions are commented out to avoid any awkward, annoying errors.

Save the file. The rerun **AAA_Master_MeltPlot_Petrogen.m** , select option [1] again, but this time when asked, instead of entering 'N', press any key to actually run the code. It will then confirm both the name of the folder and filename to save the results, and press any key to continue. The melting model code will now run! It will display a few pieces of info while running, i.e., it will alert you when a new model is run (remember, there are 6 in this case). When the code is finished, it will make a few figures—they are currently mostly useless for isobaric batch melting, but you can look at them anyways.

Step 2: Extracting Melts

A. Now define and name melting models that you wish to eventually plot with the same symbols/colors in Excel. You are not establishing the colors in this step (that happens in Step 3), you are only finding and naming the models. Step1 should have opened the Excel file BBB_Step2_ExtractGroups.xlsx that you will use. Navigate to the sheet *SingleIsobaric*. Here you can see that Step2 models are defined between the rows tagged by "FirstTargetName" and "LastTargetName". Step1 created a huge matrix will all the different types of melts combined – but tagged them. This step tells MATLAB how to find groups of melting models by identifying models with chosen parameters. That is, the 6 isobaric batch melting models we want to plot can be found by

defining the porosity, pressure of melting (in this case the "MeltExtractedPb"), water content, bulk composition, and TYPE. **_In truth, because in Step 1 we only ran a single water content, porosity, and bulk composition, we do not need to specify these values (i.e., these columns are not needed and could be deleted). HOWEVER, you may want to run other Step1 models that vary across those parameters (e.g., compare to a DMM major element mantle source) so we will leave them as is._**.

The headings are somewhat self-explanatory, except for "Type". There are three "TYPES" of melts:

Type = 50015 are pooled melts (PM)
Type = 1115741175 are near-fractional melts (IM)
Type = 45 are "**significant melts" (SM)**. SM are the 11 important melt compositions produced along a single melting model: the first, average, and last near-fractional melts in the garnet, spinel, and plagioclase stability fields, and the on axis and the fully pooled melts.

For isobaric batch melting, we need to use the near-fractional melts (these are the near-fractional melts with an extraction porosity of 1), so the "TYPE" column is all set to 1115741175. The other types in this case are useless.

B. Now open **AAA_Master_MeltPlot_Petrogen.m**. Make sure the variable that tells the program which sheet(s) to extract melts from, "ExtractedMelts_TabNames_all" (somewhere around Line 30), is set to:

```
ExtractedMelts_TabNames_all={'SingleIsobaric'};
```

C. Now run **AAA_Master_MeltPlot_Petrogen.m** and select option [2]. It will confirm the filename and subfolder for saving, as well as the sheet names ("ExtractedMelts_TabNames_all"). It will also confirm the metlings models. Press enter (or whatever you want) each time to continue until the program runs and exits.

Step 3 Plotting Melts

A. Go back to the sheet *SingleIsobaric* in BBB_Step2_ExtractGroups.xlsx. Now look at the needed Step3 parameters:

DATANAME
TESource
FC?
Spider?
MarkerSymbols
LineWidth
ColorLine
MarkerEdgeColor
MarkerFaceColor
MarkerSize
FCLineColor

If helpful, MATLAB accepts:

Line Style	Description	Marker	Description	Marker	Description
-	Solid line	o	Circle	s	Square
--	Dashed line	+	Plus sign	d	Diamond
:	Dotted line	*	Asterisk	^	Upward-pointing triangle
-.	Dash-dot line	.	Point	v	Downward-pointing triangle
		x	Cross	>	Right-pointing triangle
		_	Horizontal line	<	Left-pointing triangle
		|	Vertical line	p	Pentagram
				h	Hexagram

Check out "**ColorsHERE.m**" for color name options and to add new ones.

Feel free to change the colors or symbols, but you don't have to.

B. When ready, open **AAA_Master_MeltPlot_Petrogen.m** and confirm that the corresponding Step 3 parameters are set to:

```
ExtractedMelts_TabName = 'SingleIsobaric';
DATANAME = 'WalterComparison';
whichPrimarySM2plot=[1:11];
whichFractionatedSM2plot= [1:11];
name4edits='';
```

The values in *whichPrimarySM2plot* and *whichFractionatedSM2plot* tell the plotting scripts which of the 11 SM to plot—if there are any SM being plotted. In this case we are not plotting SM, so these are just dummy values.

C. Run **AAA_Master_MeltPlot_Petrogen.m** and this time select [3a]. *You just confirmed the values it is asking you to check, but you can also change them now if you prefer. It will also confirm that it imported the melting symbols and colors properly…if you say no ('N') then it will exit the program and direct you the Excel sheets to fix.* Eventually it will ask you which set of figures you want to plot:

```
Which set of figures do you want to plot?
[1] Geochemical (includes F,zeta)
[2] Geochem-Geophysical (crustal thickness, spreading rate)
[3] Major-trace-isotope
[4] F v Major elements
```

Enter "4". Then **enter "1"** when it asks you if you want to compare to Walter (1998). 10 figures will be made. When it's done it will open the m-file used to make the figures. This file could use some editing too, but it works. Feel free to move the legends around or rerun the script.

D. **To close all figures but some** desired figures, use the function CAB (Close All But), by typing: "**CAB 6 8**" which will close all figures except #6 and #8.

E. **Save the open figures** by typing the command "SaveFigures". It will ask you a few questions that are self-explanatory. If helpful, I always choose PDF as saved file type, the file is still a vector-based image, and the legends are saved even when they are off the screen.

Step 4 Saving melts to a spreadsheet: Run **AAA_Master_MeltPlot_Petrogen.m** and this time select [4]. Step 4 starts out the same as Step3. This option will save models with the given DATANAME in tab of their own in a new spreadsheet. It also saves some import info in "Sheet1". The melt compositions are way over to the right (e.g., column BP) as the program keeps relevant information tagged with each melt composition. For isobaric melting, these parameters are poorly filled out. They are more relevant for polybaric melting**. The default settings will save the 6 models in a new file called "Results_Petrogen_SingleIsobaric_DATANAME_WalterComparison" in the folder "Step2_ExtractedModels".** If you only wanted to save some of the 6, then change the DATANAME tag and rerun.

Polybaric near-fractional melting

There are many examples in the software that remake Figures 7–14 from Step 1. To do this, go through Steps 1–4 uncommenting and changing the code to reflect the melting conditions needed for the figures.

Step 1 Modeling Melts: Uncomment any of the polybaric melting conditions in **AAA_Step1_INFILE.m.** Comment all other models. Run **AAA_Master_MeltPlot_Petrogen.m** and choose option 1

Step 2 Extracting Models.

A. Inspect BBB_Step2_ExtractGroups.xlsx. Tabs/Sheets refer to similarly grouped melting models, e.g., :
   - "SingleMeltingModels" contains subgroups of single melting models, such as *FR0.1%-Nom.Anhyd–1350C–#8–1cm/yr.*
   - "Bulky" does not restrict major element bulk composition, so each subgroup contains 31 melting models, e.g., *FR0.1%-Nom.Anhyd–1350C–1cm/yr*. This tab is used to make Figure 9–11.

   All models between **FirstTargetName** and **FirstTargetName** will be exported from Step1.

B. Check that the right Excel sheets for Step2 are uncommented in variable "ExtractedMelts_TabNames_all" (somewhere around Line 30). They should be:

```
ExtractedMelts_TabNames_all={'Figs5and6','Bulky','FigS2andS
3','SingleMeltingModels','Fig5','Fig6'};
```

   By defining multiple Tabnames, you will be re-extracting the models listed in the given Tabnames. Feel free to delete any tabnames from

`ExtractedMelts_TabNames_all` that you have not edited or changed, if you prefer.

For polybaric melting, you will likely want to designate the three different "TYPES" —near-fractional (IM), pooled (PM), or significant melts (SM)—as their own models, even for a single melting model. This is because we typically wish to plot these different melt types as unique symbols in Step 3, and so each melting type needs its own line, as shown in the examples.

When ready, run **AAA_Master_MeltPlot_Petrogen.m** and choose option 2 and go through all the prompts.

Step 3 Plotting

A. Open **AAA_Master_MeltPlot_Petrogen.m and** edit the following variables to reflect the figure(s) you want to make e.g., :

```
ExtractedMelts_TabName = 'Fig6';
DATANAME = 'Fig6';
whichPrimarySM2plot=[1:11];
whichFractionatedSM2plot = [1:11];
name4edits='';
```

B. Run **AAA_Master_MeltPlot_Petrogen.m** and choose option 3a (or 3b if you want to keep making figures with the same parameters you already have loaded). Follow all the prompts. If you designated any "SM" to be plotted, you will be asked to confirm with how their symbols appearance, note that these symbols WILL NOT APPEAR IN THE LEGENDS.

C. Choose which sets of Figures you want to make…currently your options are :

```
Which set of figures do you want to plot?
[1] Geochemical, includes F,zeta (e.g, Figs 7,8,9,10)
[2] Geochem-Geophysical (crustal thickness, spreading
rate,(e.g.,Figs 5,6,11)
[3] Major-trace-isotope (Figs 12-14)
[4] F v Major elements
```

Each "option" runs a different m-file that all, by themselves, makes a variety of figures. In general, I've tried to organize new styles of plots by numbering up to the next tens digit. I.e. in *"Step[3]-[1] Geochemical, includes F,zeta (e.g, Figs 7,8,9,10)"* major element oxide plots would be Figures 1-10 (but only Figure 1 currently exists), trace element ratio diagrams are Figures 20-30 (but only Figures 20 and 21 exist), Spider diagrams are Figures 30-40, etc…. That way if you want to make a new version of Figure 1 but with different elements, you can make a copy of Figure 1 and then define it as Figure 2, which keeps like-figures near each other.

D. If you want to edit a figure, navigate to the figure in question in the proper .m files (the code will tell you which script it in in, and also open the file). Find the code to edit a figure (e.g., modify axes, change the elements being plotted, make a new version of the code) by searching for the figure number. I.e.,

search for "**Figure(20)**" in "**ddd_Step3_GenericFigures.m**" to modify the trace-element ratio diagrams. If all you want to do is change the axes, you can do this in a separate file as shown for the example paper figures (Step 5).

F. **To close all figures but some** desired figures, use the function CAB (Close All But), by typing: "**CAB 6 8**" which will close all figures except #6 and #8.
G. **Save the open figures** by typing the command "SaveFigures". It will ask you a few questions that are self-explanatory. If helpful, I always choose PDF as saved file type, the file is still a vector-based image, and the legends are saved even when they are off the image.

Step 4 Saving melts to a spreadsheet: Same directions as for isobaric batch melting.

NOTES:

- There are lots of other details in using this code, especially in plotting. Please contact me with questions so that I can help you and also improve this document and the code (as it can be cleaned up significantly). Hopefully, one day, other melting models results (e.g., pMELTS) will easily be compared to Petrogen results using this software.

- The functionality to run the polybaric melting model without the geodynamic model, by entering your temperatures and upwelling velocities either as a column or a grid, has not yet been implemented—but is easily made possible. Contact me for help!