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Please contact us by email with problems, queries, or comments

Welcome to the OPAM thermobarometer for igneous rocks at crustal pressures (0.5 – 10 kbar) saturated in Olivine + Augitic clinopyroxene + Plagioclase ± oxides.

Basic Setup

The running of this model requires two pieces of software which are extremely easy to install, are very stable, and are completely free. These are: R (https://cran.r-project.org/) and the attractive user interface RStudio (https://posit.co/download/rstudio-desktop/). Once R and RStudio are installed, opening RStudio will automatically open and run R, meaning that all scripts and user inputs are performed entirely through RStudio (R remains in the background and you do not need to worry about it or interact with it following its installation). You will also need a method to open and edit a CSV file (Excel, for example) which is to be populated with melt or bulk rock data in oxide wt%. The model is designed to be executed using the click of a single button in RStudio (source; top right of script panel in RStudio) and so no prior coding knowledge is required aside from basic computer literacy.

The folder **OPAM_UserInput** needs to be placed in its entirety somewhere sensible on your computer. Sometimes OneDrive can cause a bit of a pickle, so it is best to save it somewhere local like your documents folder if possible. Do not delete or rename anything in this folder.

The output of the calculation (**UserOutput_*DateAndTimeYouRanIt*.csv)** is saved inside this folder once you have executed the code. You may move it once it is saved to any directory of your choosing. As this output file has a unique name, running the code repeatedly will save a new copy each time in the **OPAM_UserInput** folder so no output file is ever overwritten. An identical .Rdata file is also saved with the same name.

Running the Code

As a first pass, please do think logically about the compositions you are putting into the model. Are they reasonably likely to be saturated in the phase assemblage? Can you verify this petrographically? Are there any other independent tests you can perform to confirm or deny saturation? Using models "blind" is not to be advised if good scientific conclusions are to be drawn from output data. The original rock is always the best source of this information.

For a reasonable set of melt compositions perform the following steps:

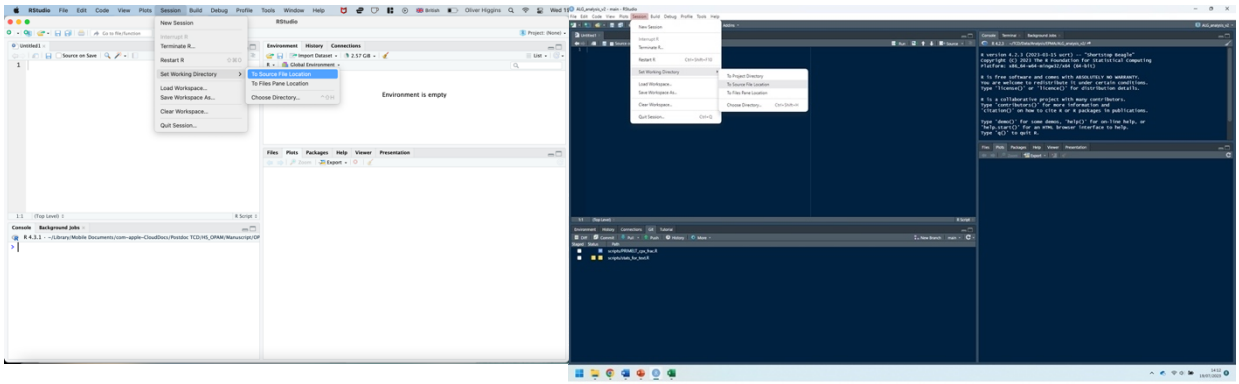
1) Populate the **UserInput.csv** spreadsheet with your natural data. All Fe as FeO. If the oxide is not present in your melt/magma leave blank. Numeric values only (not NA, bdl etc.) We have added all the oxide columns that the code accepts to the **UserInput.csv** template. You can also add as many sensibly named additional columns that you desire which can contain text (localities etc) or numbers (trace elements etc). These will be retained in the output file and the code will automatically detect the oxide columns to work with.

Note: These oxide data can be normalised to 100 wt% but the code will also do this by default (and output the normalised result), so it is not fundamental. The ***UserInput.csv*** *is by default populated with 2015 Wolf Volcano data which we use for benchmarking in text, so just delete these data and populate with your own values. Do not change the file format from csv to xlsx.*

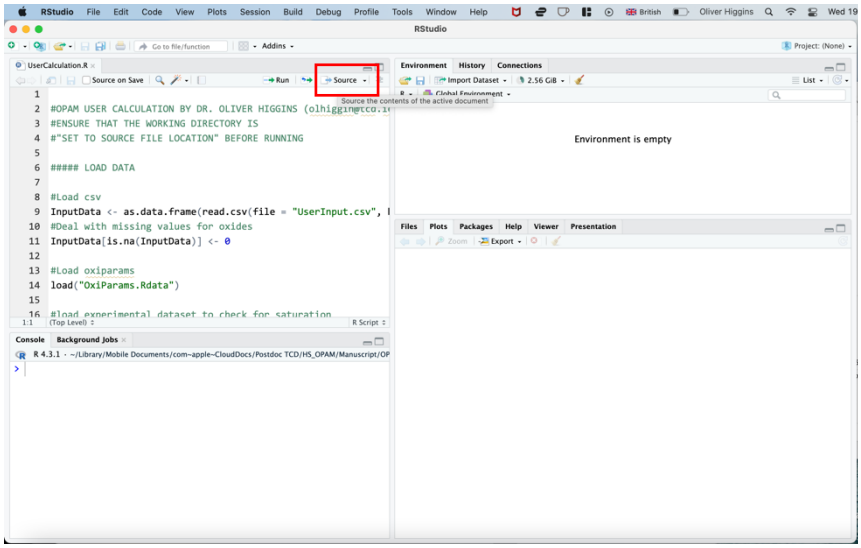
2) Open the script **UserCalculation.R** in RStudio.

   Note: You may need to right click, select "Open With" (or equivalent) and manually select RStudio as the programme to open the file with on the first occasion that the file is opened. The easiest method is to configure your computer so that all .R files are opened with RStudio in future.

3) Set the working directory to source file location. This is so that the R script knows where the code folder is located on your computer and where the output should be saved. The example of how to do this on a Mac (left) and PC (right) are below. Use Session (top bar) –> Set Working Directory –> To Source File Location



4) Click Source (see picture below, red box). Feedback will appear in the console as the code runs.



Note: Theoretically no error messages will appear, and the code will run to its conclusion very quickly (seconds to a minute). We predict the main source of error may be a user not setting the working directory (see Step 3). The reason that the code may take more than a few seconds to run is that the saturation test relies on a distance matrix (see manuscript for details) which are quite laborious to construct and require significant memory when large. Therefore, if you are doing several hundreds or thousands of melt compositions it may be best to split into a few batches to prevent hanging issues. Perhaps test with our Wolf Data first to verify the code is working smoothly on your personal setup. There are solutions to enable faster construction of distance matrices in R, but we opted against these to avoid requiring the user to download numerous third-party packages which may create inconsistencies regarding version of R, RStudio etc. For implementation of large datasets with this code, feel free to contact us.

5) The script will automatically save your output in csv and .Rdata format (**UserOutput_*DateAndTimeYouRanIt*.csv**). This file contains: the normalised wt% values of your data; the calculations of liquid components following Table 1 of Putirka (2008); which data satisfied the OPAM convex hull test (TRUE or FALSE); the saturation probability (P_{sat}); a description of the melt according to our saturation checks (State, either SAT or UNSAT); the calculated pressure and temperature.

   *Note: the pressure and temperature are calculated irrespective of whether the melt is OPAM-saturated. To remove the melts which are not OPAM-saturated, according to our test, just filter or delete any row in the **UserOutput** spreadsheet which has "UNSAT" in the "State" column (P_{sat}<0.5). The reason we do this is so that the user can override our saturation test if they have petrographic or geochemical information which is at odds with the saturation probability. Further, it forces a user to look at the data and inspect the results. Finally, it retains the structure of your data so you can bind it with other geochemical outputs with ease. If the melt does not satisfy the OPAM convex hull test (see "InOPAMchull" column in **UserOutput.csv**), however, we strongly advise to consider it unsaturated. For any row in which "InOPAMchull" is listed FALSE, the "State" column in **UserOutput.csv** will be set to UNSAT by default regardless of P_{sat}.*