

Readme for Apatite Crystallisation model Graphical User Interface

1 Overview

The model is built on that published by Humphreys et al. (2021) and allows users to model the behaviour of CL, F and OH in apatite, melt and fluid during fractional crystallisation and volatile exsolution. It also incorporates sensitivity analysis to explore how different conditions could have resulted in the observed apatite compositions.

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How to cite this model:

Lormand, C., Humphreys, M.C.S., Coumans, J.P., Colby, D. J., Chelle-Michou, C. & Li, W. Volatile budgets and evolution in porphyry-related magma systems, determined using apatite. Submitted to Lithos (2023).

1.1 Updates from previous version

- Temperature-dependent KD values are incorporated (using the method of Li and Costa, 2020).
- Temperature can be treated in several different ways. It can be kept constant at a temperature set by the user. The user can upload a temperature melt fraction (TF) curve, or a pseudo-TF Curve can be generated using the approach of Huber et al. (2010).
- The H₂O saturation value is now incorporated within the multistart routine.
- Salinity calculations have been incorporated to provide the user information on the aggregate amount of NaCl_{eq} in the fluid phase (following equation 13 of Tattich et al. 2021) and the quantity of NaCl in the fluid at each fractionation step (for the target curve only).
- The code has been incorporated into a graphical user interface, allowing easy input and data extraction. This is available as a MATLAB application or a Standalone application.
- Included a Data Explorer allowing users to plot their data to help inform the direction of the trends.
- The underlying code has also been updated and is available to download.

2 System Requirements

This model has three versions: a MATLAB app, a standalone application, and an editable MATLAB script.

- The multistart routine is computationally intensive and should be run using parallel processing across multiple CPU cores. Ideally, a computer with a minimum of 10 cores should be used. The model will run on a laptop with six cores; however, run times will be significantly higher,

and the computer may crash if other tasks are being completed simultaneously while running the multistart.

- The application is compatible with both Windows OS and macOS.
- If using the MATLAB app or MATLAB script, the following MATLAB packages are needed:
 - MATLAB 2021 or later (Only necessary for the MATLAB app).
 - MATLAB optimisation toolbox
 - MATLAB Global optimisation toolbox
 - MATLAB Parallel Computing Toolbox
- If using the standalone version, MATLAB Runtime 2023 is required.

3 Using the model

It is **highly recommended** that users use the MATLAB app as this provides the easiest way of using the model and helps reduce the potential for errors in setting up model runs. The MATLAB script should only be used if there are specific areas of the code users wish to edit. Editing the code may result in the model breaking.

The interface for the MATLAB app and the standalone application is identical; however, the standalone application has limitations in handling figures and cannot use parallel processing. Section 7 outlines these differences and the additional steps needed to export figures.

Files created using the MATLAB script are compatible with the MATLAB app; however, information on the upper and lower Multistart bounds, number of start points and tolerance values are not included.

Files can also be shared between different users using the method outlined in Section 8.

3.1 Installing the model

3.1.1 MATLAB Application

- Open MATLAB (2021 or later)
- Download the '**Apatite Crystallisation Multistart. mlappinstall**' file.
- Double-click on the .mlappinstall file.
- A dialogue box will appear in MATLAB asking if the user wishes to install the file in Apps. Click install.
- Once installed, navigate to the Apps tab in MATLAB and click on the **Apatite Crystallization Multistart** app to launch.

3.1.2 Standalone Application

- Download MATLAB runtime 2023a from [MATLAB Runtime - MATLAB Compiler - MATLAB \(mathworks.com\)](https://www.mathworks.com/matlabruntime)
- Download the **ApatiteCrystallisationMultistart.exe** file.
- Install MATLAB runtime.
- Double-click on the **ApatiteCrystallisationMultistart.exe** file to run the application.

3.1.3 MATLAB Script

- Download the .m script and save it to the folder which contains the apatite molar ratio data.
- It is highly recommended that a separate copy of the script is used for each model run to avoid overwriting data and save the parameters used for the multistart.
- Double-click on the .m script to open it in MATLAB.

3.2 Setting up a model run

- Once the application has loaded, the graphical user interface will be displayed (Figure 1).
- Provide the model run a unique name (Figure 1 [1]).
- Click on **Load Data File** (Figure 1 [2]) and navigate to the .csv file that contains the apatite volatile ratios. This file must contain Cl/OH, F/OH and F/Cl ratios (See example layout below).

Label	Phase	P2O5	CaO	MnO	SiO2	MgO	FeO	La2O3	Ce2O3	F	Cl	SO3	OH	Cl/OH	F/OH	F/Cl
AP_1																
Ap_2																
AP_3																

- The path to this file will be displayed in the adjacent box (Figure 1 [2]). This is the directory in which an output folder will be created. The name of the .csv file will be displayed in the **Data File** box (Figure 1).
- Specify a name for the output folder where all data files will be saved (Figure 1 [3]). This folder will be created in the set directory.
- Provide a name for the target file (Figure 1 [4]). See Section 5 for information on how output files are named.
- Decide how to deal with temperature by clicking the drop-down menu (Figure 1 [5]).

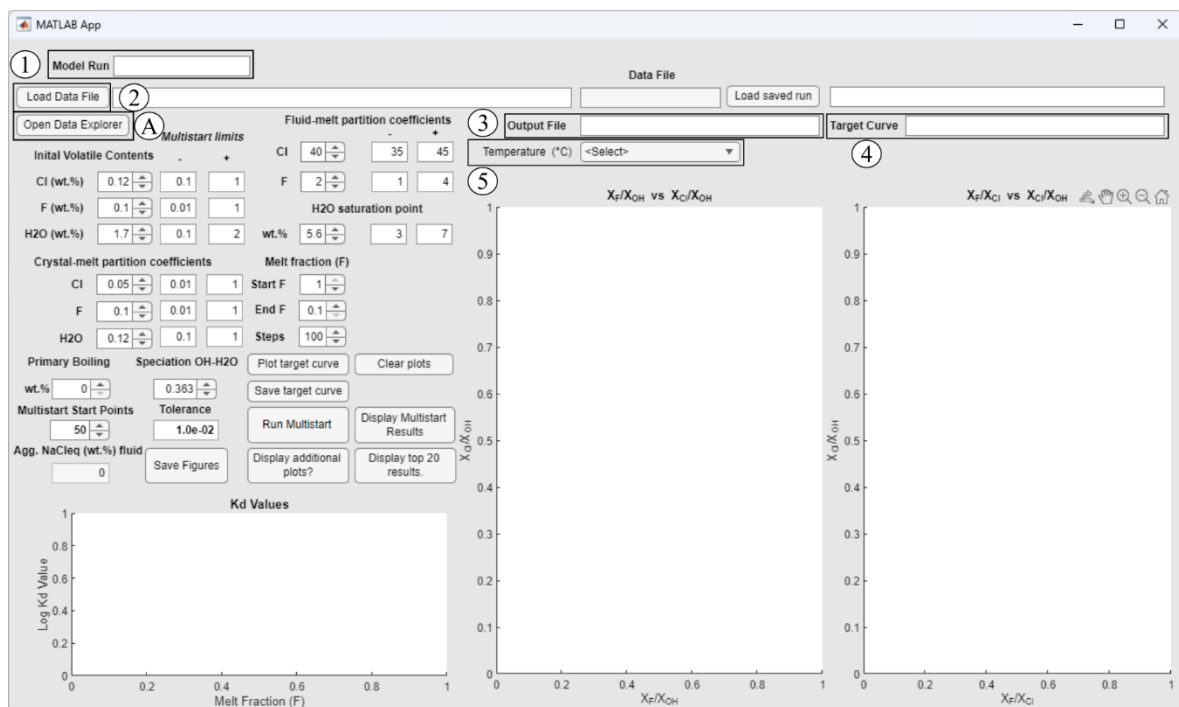


Figure 1: Overview of MATLAB app graphical user interface. 1) Input name for the model run. 2) Click to load molar ratio apatite data. 3) Name of the output file. 4) Give the name of the target curve. 5) Select a method of dealing with temperature.

3.2.1 Temperature

There are currently three ways of dealing with temperature.

- User sets a temperature value that is kept constant throughout the model.

- The user loads a temperature melt fraction (TF) curve specifying the temperature at a given melt fraction.
- The user can generate a pseudo-TF curve using the approach of Huber et al. (2010).

The user must select an option from the drop-down menu (Figure 2).

Temperature is a critical variable as it greatly influences the calculated Kd values (see Li and Costa (2020) for more details on calculating Kd values). When using TF curves, minor adjustments in the temperature profile can drastically alter the shape of the target curve. Therefore, careful consideration should be given to the values used and, where possible, these should be informed by independent temperature estimates.

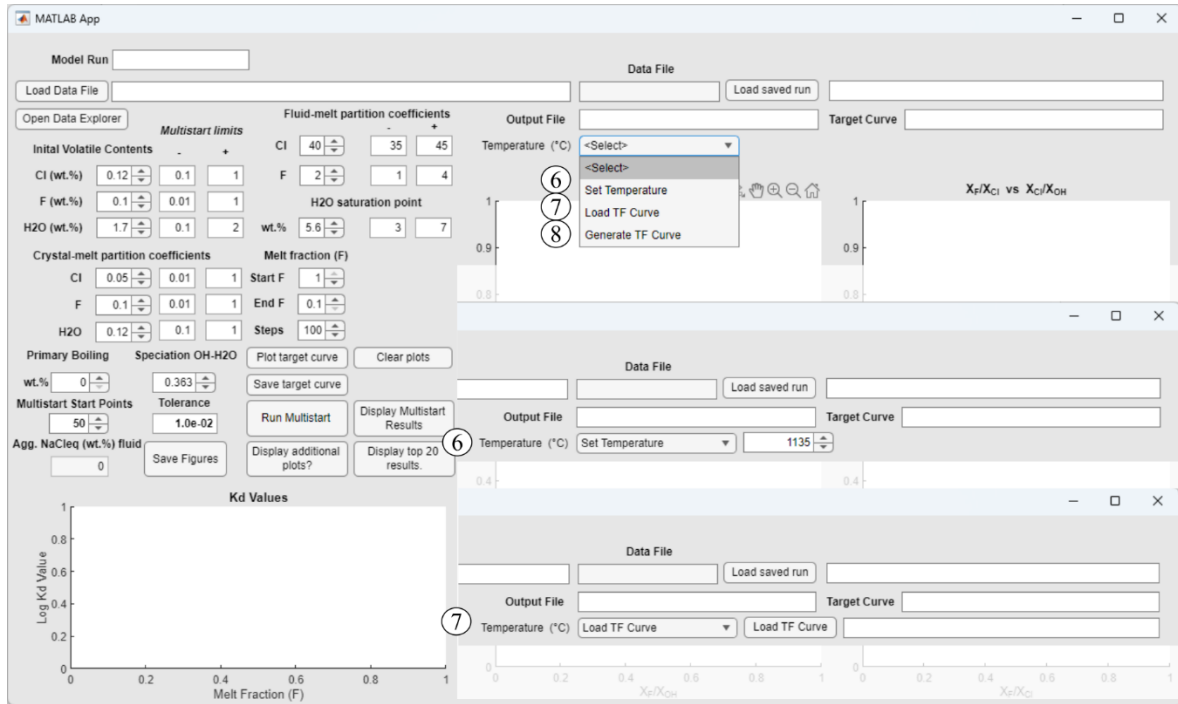


Figure 2: Overview of the ways to select temperature. 6) Set a constant temperature. 7) Load a Temperature Melt fraction (TF) Curve. 8) Generate a pseudo-TF curve.

3.2.1.1 Set Temperature

A box will appear where the user can enter a temperature in °C (Figure 2 [6]). This must be between 500-1500 °C.

3.2.1.2 Load TF Curve

- Click the **Load TF Curve** (Figure 2 [7]) button and navigate to the .csv TF File.
- This file must have temperature in °C in the first column and melt fraction in the second with no column headings.
- The path to this file will appear in the box marked in Figure 2 [7].

3.2.1.3 Generate TF Curve

Generating a pseudo-TF curve uses the approach of Huber et al., 2010 (Equation 1).

$$F = \left(\frac{T - T_{sol}}{T_{liq} - T_{sol}} \right)^b \quad (1)$$

Where F is the melt fraction, T_{liq} is the liquidus temperature, T_{sol} is the solidus temperature and T is the temperature at the given step. The temperature steps are determined by dividing the difference between the liquidus and solidus temperature by the number of crystallisation steps the user sets. 'b' is a free parameter used to set different crystallisation behaviours. Figure 4 shows examples of how varying b produces different TF curves. As b approaches 0, the magma will crystallise over a narrow temperature range close to the solidus.

- Three new options will appear (Figure 3 [8b])
- Give a name to this pseudo-TF Curve (Figure 3 [8a])
- Set a liquidus temperature (T_{liq}), a solidus temperature (T_{sol}) and a value for b . See Huber et al. (2010) for more information on the b parameter.
- The model is susceptible to changes in temperature. Therefore, robust values must be chosen. When plotting target curves (see section 3.2), these values can be changed to see how they affect the generated target curve.
- To save a pseudo-TF curve, click the **Save TF Curve** button (Figure 3; 8c).
- It is advised that the user plots the target curve with the pseudo-TF curve before saving (see section 3.2: Plotting a target curve).

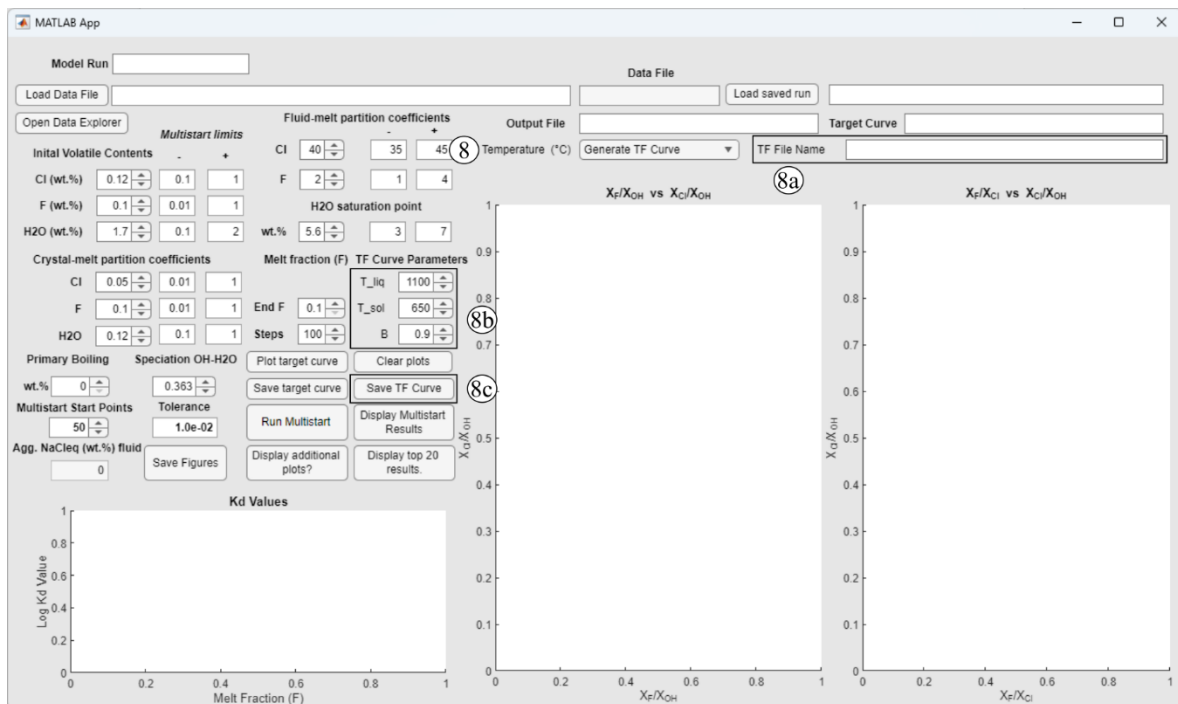


Figure 3: Overview of user inputs to generate a pseudo-TF Curve. 8) Select 'Generate TF Curve'. 8a) Provide name for pseudo-TF .csv file. 8b) Select the appropriate liquidus temperature (T_{liq}), solidus temperature (T_{sol}) and b parameter (see Figure 4). Once a pseudo-TF curve has been generated, click Save TF Curve (8c).

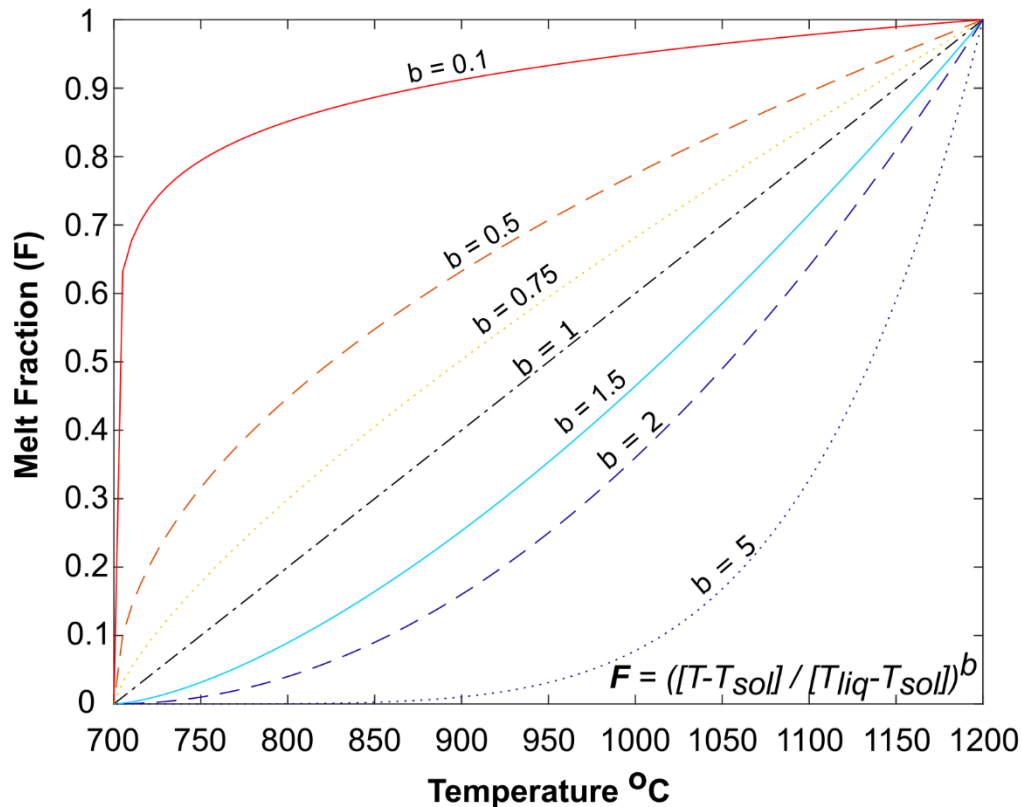


Figure 4: Overview of how varying the b parameter in Equation 1 (Huber et al., 2010) influences the shape of the pseudo-TF curve.

3.3 Plotting and saving a target curve

Once a model run has been set up, a target curve must be fitted to the apatite data. The petrology should inform the direction of this target curve (e.g., the target curve should start at the least evolved point, which can be constrained by looking at apatite inclusions in early crystallising phases. You can use the **Data Explorer** to help inform the direction of your trend). The results of the Multistart runs will then be compared to this curve to find the best-fit parameters.

1. Enter the desired start parameters in the highlighted fields (Figure 5) and click **Plot target curve** (Figure 5 [9])
2. Three plots will now be generated.
3. The first shows changes in log Kd values as the melt fraction reduces (Figure 5 [10]). The second shows X_{Cl}/X_{OH} vs X_F/X_{OH} , and the third shows X_{Cl}/X_{OH} vs X_F/X_{Cl} (Figure 5 [11 & 12]).
 - These plots are fully interactive, so the user can zoom in and pan to inspect the curve.
4. If the curve provides a good fit, skip to section 3.3.
5. It is likely that the first target curve will not provide a good fit. Therefore, edit the initial parameters (Figure 5) and click **Plot target curve**.
 - It is usually the case that multiple attempts at fitting a target curve are needed through trial and error to find a good fit.
6. To learn how each parameter influences the curve, changing a single parameter and then replot the data to compare the two curves is advised.
7. Multiple curves can be plotted at the same time for comparison.
8. To reset the plots, click **Clear plots**.

9. It is essential to ensure that the values chosen for the different parameters are realistic; for instance, the fluid melt partition coefficients for Cl are generally expected to be higher than for F (e.g. Cassidy et al. 2022).
10. When plotting the target curve, the aggregate amount of NaCl_{eq} in the fluid is also calculated and displayed (Figure 5 [13]). The instantaneous amount of NaCl_{eq} in the fluid at each fractionation step will be saved in the target curve file.
11. Once a good fit has been achieved, click **Save target curve**.
12. This will generate and save a target curve based on the values currently displayed on the interface.
13. If a pseudo-TF curve has been used, now is the recommended point to save it.
 - Through the iterative process of fitting a target curve, it may be necessary to edit the temperature to achieve a good fit.

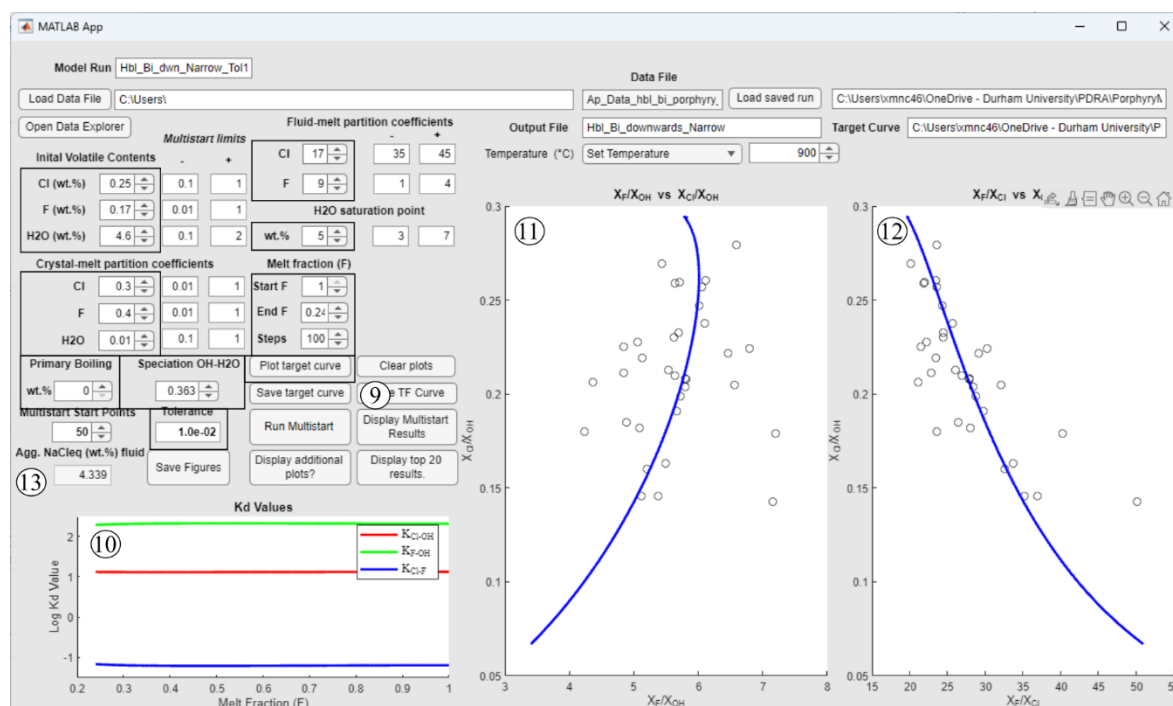


Figure 5: Overview of plotting a target curve. Input initial start parameters for the target curve in highlighted boxes and then click **Plot target curve** (9). This will display how the K_d values vary with melt fraction (10) and the target curves in the two molar ratio plots (11, 12). The initial start parameters can be varied, and the data replotted with the target curve for comparison. Once a suitable target curve has been generated, click **Save target curve**.

3.3.1 Note on H_2O_i and $\text{H}_2\text{O}_{\text{sat}}$

When plotting a target curve or running the Multistart routine, the initial H_2O value must be less than or equal to the $\text{H}_2\text{O}_{\text{sat}}$ value so that the melt is not oversaturated at step 1. When plotting a target curve, if the H_2O_i value is greater than the $\text{H}_2\text{O}_{\text{sat}}$ value, a warning will appear, and the $\text{H}_2\text{O}_{\text{sat}}$ value will be set to H_2O_i value. The same thing happens within the Multistart routine. If the chosen H_2O_i value is greater than the chosen $\text{H}_2\text{O}_{\text{sat}}$ value, then the $\text{H}_2\text{O}_{\text{sat}}$ value will be set equal to the H_2O_i value.

3.4 Running the Multistart routine

Once a target curve has been saved, a multistart run can be completed.

1. Firstly, set upper and lower limits for each start parameter. The multistart routine will test multiple start points between these two values.
2. The lower limit must be less than the upper limit. If this is not the case an error is produced.
3. Initially, it is recommended to set wide limits for the multistart to search between, to prevent the user from biasing the model towards the predefined values. The algorithm can then be re-run with narrower bounds based on the results of the initial run.
4. Set the number of start points for the multistart to test (Figure 6 [14]). The more start points, the longer the multistart will take to run. It is recommended to run at least 400 + start points.
5. Set the tolerance for the multistart routine (Figure 6[15]). The default value is 1×10^{-2} . This is the tolerance at which the solver considers two solutions equal. To see more solver runs, set the tolerance value to a lower value (i.e., 1×10^{-12}). Setting the tolerance to a lower value will result in more runs being displayed. However, it will take significantly longer to run the multistart.
6. Ensure that all the limits, number of start points and tolerance values are correct and then click **Run Multistart** (Figure 6 [16]).
7. A progress bar will appear on the screen, showing that the multistart is running. This will disappear once the multistart run is complete.
8. Once the run is complete, a .mat file and a .csv file will be saved in the output folder containing all the results.

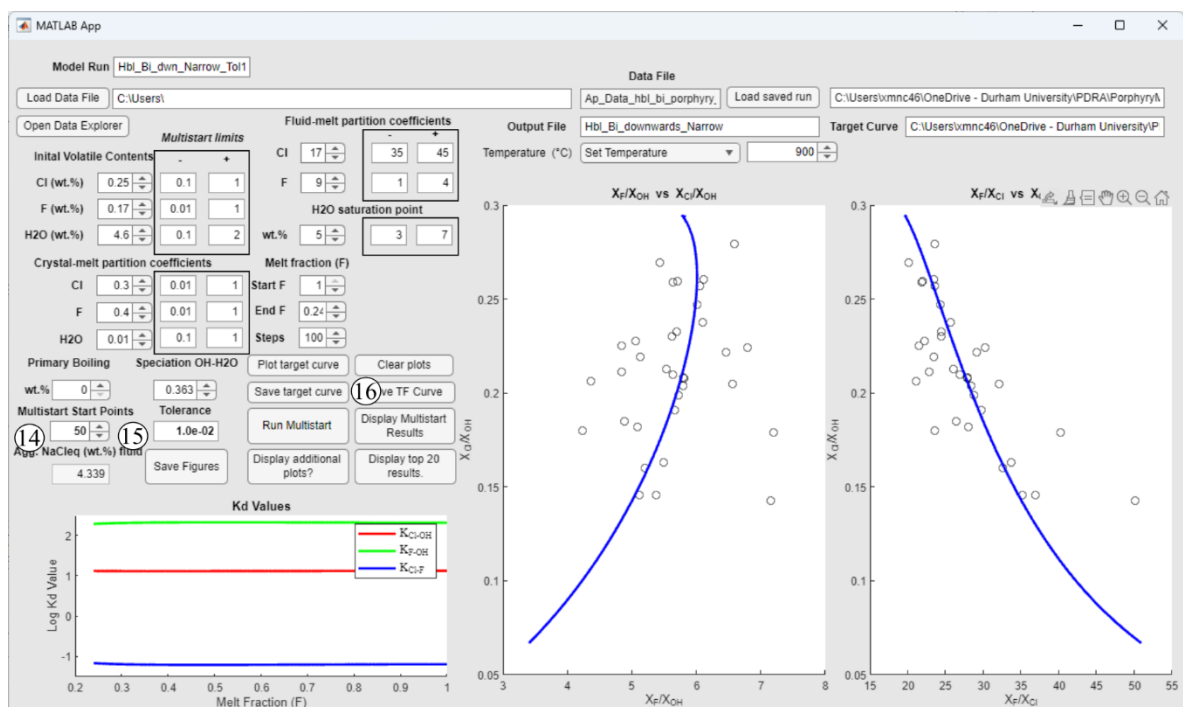


Figure 6: Once a target curve has been saved, the upper and lower bounds for the multistart model (highlighted). Select the number of start points (13) and tolerance value, then click **Run Multistart** (14).

3.5 Display Multistart Results

1. To display the Multistart results, click either **Display Multistart Results** (Figure 7 [17]) or **Display Top 20 results** (Figure 7 [18]).

-
- MATLAB App**
- Model Run** Hbl_BI_dwn_Narrow_Tol1
- Data File**
 Ap_Data_hbl_bi_porphyry, Load saved run C:\Users\vmnc46\OneDrive - Durham University\PDRA\PorphyryA
- Output File** Hbl_BI_downwards_Narrow **Target Curve** C:\Users\vmnc46\OneDrive - Durham University\IP
- Fluid-melt partition coefficients**
- | | - | + |
|----|----|----|
| CI | 17 | 35 |
| F | 9 | 1 |
- Multistart limits**
- | | - | + |
|---------------------------|------|---|
| Initial Volatile Contents | 0.25 | 1 |
| F (wt.%) | 0.17 | 1 |
| H2O (wt.%) | 4.6 | 2 |
- H2O saturation point**
- | | - | + |
|------|---|---|
| wt.% | 5 | 3 |
- Crystal-melt partition coefficients**
- | | - | + |
|-----|------|---|
| CI | 0.3 | 1 |
| F | 0.4 | 1 |
| H2O | 0.01 | 1 |
- Melt fraction (F)**
- | | - | + |
|---------|------|---|
| Start F | 1 | |
| End F | 0.24 | |
| Steps | 100 | |
- Primary Boiling** **Speciation OH-H2O**
- | | - | + |
|-----------|----|---------|
| wt.% | 0 | 0.363 |
| Tolerance | 50 | 1.0e-02 |
- Agg. NaCl eq (wt.%)** 4.339
- Multistart Start Points**
- Display additional plots?** **Display top 20 results.**
- Kd Values**
- log RMSE**
- XF/XOH vs XC/XOH**
- XF/XCI vs XC/XOH**

Figure 2 displays five histograms showing the distribution of model coefficients. The histograms are for H_2O wt. %, Cl wt. %, F wt. %, D_{xs-m} Cl, and D_{xs-m} F. The distributions are generally unimodal and centered around 0.2, 0.3, 0.2, 0.2, and 0.2 respectively.

Figure 8: Overview of additional plots generated by the MATLAB app. Left) Histograms showing the distribution of initial values chosen by the Multistart solver. Right) Scatter plots showing the RMSE of each of the successful runs. This is a helpful plot for deciding how to narrow the limits for the multistart solver.

3.6 Saving Figures

1. To save figures displayed within the application, click the **Save Figures** button (Figure 7 [20]).
2. Choose which figures to save: **All the multistart results**, the **top 20 results** or the **target curve** (Figure 9).
3. If the **Top 20 results** are selected, an additional dialogue box will appear for the user to set if the colour bar is scaled to the top 20 results or the whole dataset.
4. A figure will be generated in a separate window.
5. Click View > Property Inspector to open the inspector panel. This allows the user to change the figure's colours, axis limits and text by clicking on the graph they wish to edit (Figure 10).
6. Once happy with the figure, click file > Export setup.
7. Make any changes, click **Apply to figure** and then **Export**.
8. Navigate to the output file, name the figure, and select the file type to save it.
9. If the user wishes to save the additional plots, click **Display additional plots** and View > Property Inspector.
10. Make any changes to the figure.
11. Click File > Export setup.
12. Make any changes and click **Apply to figure** and then **Export**.
13. Navigate to the output file, name the figure, and select the file type to save it.

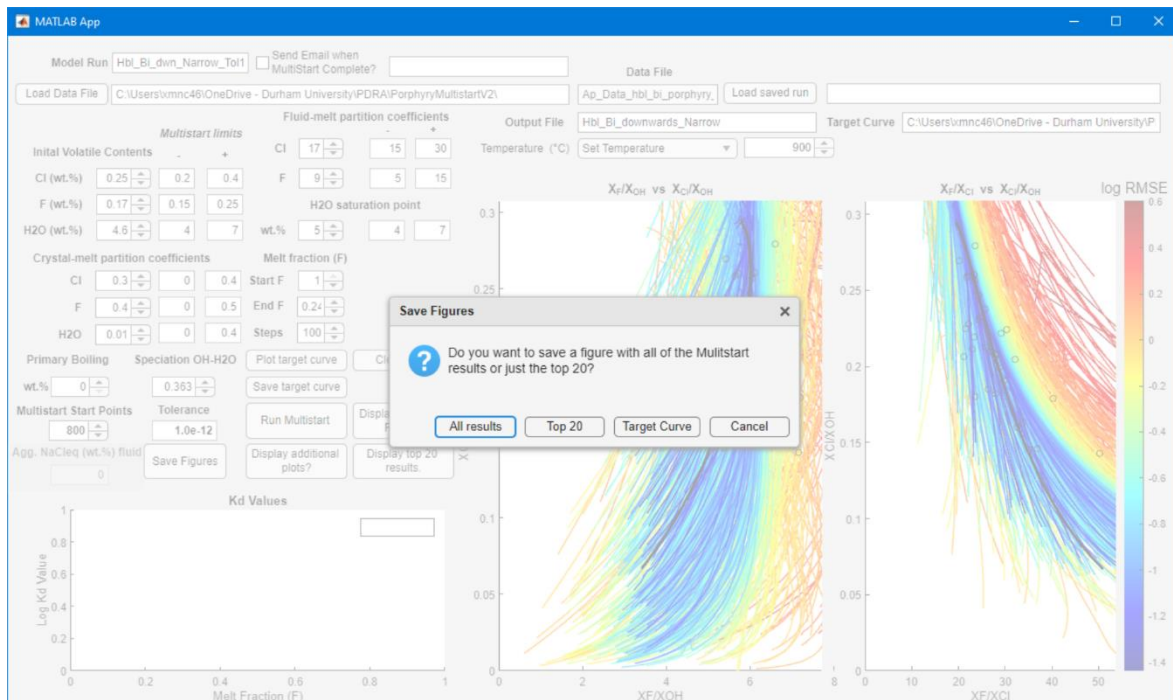


Figure 9: Once the **Save Figures** button is clicked, a choice is presented for the user to decide which figures they wish to save. A second dialogue box will appear if the Top 20 is selected, asking the user if they want to scale the colour bar to the whole dataset or just the top 20 results.

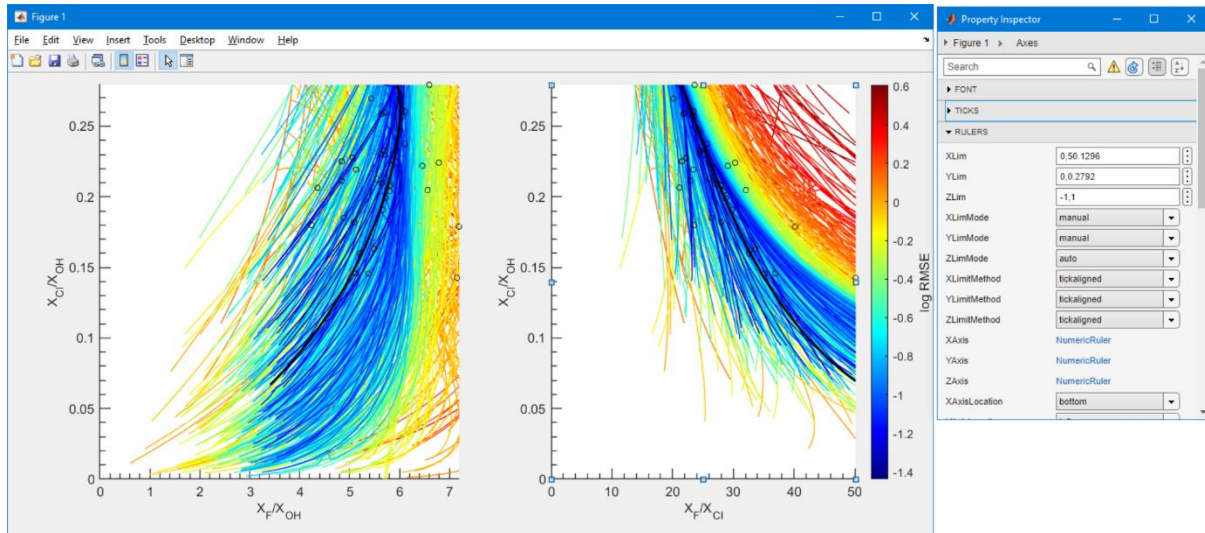


Figure 10: Example of generated figure if **All Results** (Figure 9) is selected. A separate figure will open, and the property inspector appear. The property inspector can be used to edit the figures. The user selects which figure to edit and then can make adjustments.

4 Loading a previous run

There is the option to load previous multistart runs and target curves.

- Click on **Load saved run** and navigate to the `_log.csv` file for the model run to load.
- Select this `.csv` file and click open.
- This will load all data that is associated with the model run.
- If a warning message appears, see sections 10 and 11 for details on why this happened.
- If a multistart run has been completed for this model, then the upper and lower bounds used will appear in the GUI.
- The user can then edit any of the values; however, it is **HIGHLY** recommended that the user provide a new model name and not overwrite any of this data. The application will warn the user if they try to overwrite an existing file.

5 How are output files named?

Target files: (Example in *italics*)

The user inputted the		Model run			
Directory	name for the output folder	Data file name	name	Target Name	File type
<i>C:\User\Data\</i>	<i>Output1\</i>	<i>ApatiteData_</i>	<i>Model1_</i>	<i>Tgt1</i>	<i>.csv</i>

Log files: (Example in *italics*)

Directory	User inputted output folder	Model		
		Run name	_log	File type
<i>C:\User\Data\</i>	<i>Output1\</i>	<i>Model1</i>	<i>_log</i>	<i>.csv</i>

Custom TF files: (Example in italics)

Directory	User inputted output folder	Model run		File type
		name_	TF file name	
<i>C:\User\Data\</i>	<i>Output1\</i>	<i>Model1_</i>	<i>CustomTF</i>	<i>.csv</i>

Multistart Output: (examples in italics)

Two files are saved. One is a .mat file, and the other is a .csv file. The CSV file contains the initial values for each multistart run and the root mean square error (RMSE) for that iteration.

Directory	User inputted		Data file name	Model	
	output folder	Multioutput_		run name	File type
<i>C:\User\Data\</i>	<i>Output1\</i>	<i>Multioutput_</i>	<i>ApatiteData_</i>	<i>Model1</i>	<i>.mat</i>
<i>C:\User\Data\</i>	<i>Output1\</i>	<i>Multioutput_</i>	<i>ApatiteData_</i>	<i>Model1</i>	<i>.csv</i>

6 File outputs

6.1 Target curve

The Target curve file contains a breakdown of the calculated variables at each fractionation step. This includes the variation in Kd values, the molar ratios (F/OH, Cl/OH, F/Cl) of apatite, the molar volatile contents of the melt (H₂O, Cl, F, OH) and apatite (Cl, F, OH). The incremental mass of the fluid (Fluid_inc_mass), the Molar fraction of NaCl_{eq} in the fluid (NaClEq_Fluid), the molar fraction of H₂O in the fluid (XH₂O_fluid) and the instantaneous NaCl_{eq} in the fluid in mass fraction (calculated after Tattitch et al., 2021). The aggregate amount of NaCl_{eq} (wt.%) in the fluid is displayed on the app GUI. These data will also allow users to calculate the amount of Cu in the melt and fluid using the methodology of Tattitch et al. 2021.

6.2 Log file

The log file contains all the data the user input into the GUI so it can be accessed later or loaded into the app to perform more runs. When a Multistart run has been initiated, the upper and lower bounds set by the user are also saved to this file.

6.3 TF Curve

This file contains the pseudo-TF curve generated by the user. It contains the temperature in °C and the melt fraction at each temperature step.

7 MATLAB standalone application

This standalone application should only be used if the users cannot access a MATLAB licence. This application has several limitations, which will increase the run times of the multistart. The application does provide a good tool for generating target curves.

The interface and method for loading data and running model runs are identical to the MATLAB app.

7.1 Limitations

- The standalone MATLAB application cannot use parallel processing and will take **significantly** longer to run Multistart runs. (e.g., it takes at least 4 minutes to run one start point with a tolerance of 1×10^{-12})
- In addition, users cannot edit figures using the property inspector. Users can interact with the figures and manually move axes, which can be quite fiddly. Figures can be saved similarly (File > Export Setup).

8 File Sharing

To share files between different users on different computers, it is necessary to change the `_log` file to point to the correct location of the data files. This can be done using the `SetDirectory.m` script using the following steps:

- Download all the files and folders, including raw data files (e.g. Files are downloaded and saved to file 'Example' Figure 11)
- Copy the 'SetDirectory.m' script into this file (Figure 11)
- Open MATLAB and navigate to this folder.
- In the command window type `SetDirectory()` and press Enter
- This will look through all subfolders in this folder and search for `_log` files.
- It will then change the file paths in the relevant fields to this current directory.

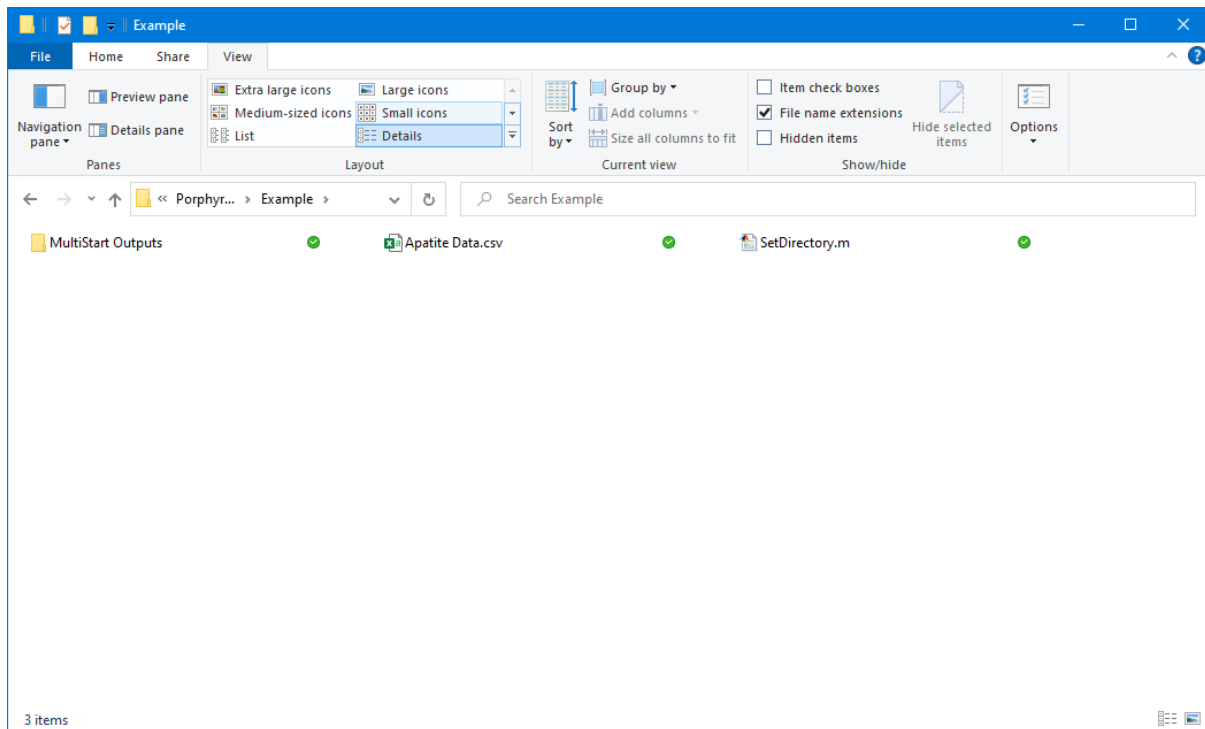


Figure 11: Example of how to save files from another user and use the SetDirectory.m script. Here, files are kept in a Folder called 'Example', and the SetDirectory.m script is copied into this folder.

9 MATLAB Script

This script should only be used by experienced MATLAB users who wish to edit the code for a specific purpose. Any edits the user makes may result in the model breaking or returning invalid results. There are no safeguards in the code to prevent users from overwriting data.

The script must be saved in the folder which contains the user's apatite molar ratio data.

For detailed instructions, see Humphreys et al, 2021.

9.1 Generate Target Curve

- Uncomment **line 48** operation = 'Explore model and/or create multistart target';
- Ensure **lines 49 and 50** are commented out.
- Provide a name for an output folder (**Line 61**)
- Provide the name of the dataset that will be loaded (**Line 62**)
- Give the model run a name (**Line 63**)
- Set temperature, either a set temperature (**Line 69**) or load a TF file (**Line 72**)
- Set the start and end melt fraction (**Lines 85 & 86**)
- Set target parameters **Lines 100 - 129**.
- Click run.
- This will generate a figure showing the apatite data and the generated target curve.
- Alter the parameters in lines 100-129 to change the curve and repeat until a good fit to the data is found.

9.2 Run Multistart to Target

- Comment out **line 48** and uncomment **line 49** operation = 'Run multistart to a target';
- Set the number of fractionation steps (**Line 152**)

- Set the number of start points for the Multistart (**Line 153**)
- Set the Tolerance (**Line 160**)
- Set the upper and lower limits for the multistart (**Lines 349-373**).
- Ensure that the upper and lower limits are greater or less than the initial values that have been selected.
- Run the script.

9.3 Visualise Multistart Results

- Comment out line 49 and uncomment **line 50** operation = 'Visualize multistart outputs';
- Type the filename to visualise in **line 175** (see Section 5 for details on naming convention of files)
- Run the script.

10 Data Explorer

A key part of defining the target curve it is determining the likely direction of any trends in the apatite dataset. To support this a Data Explorer (Figure x [A]) feature is included within the application. This allows users to load in data and plot different variables on two interactive figures. Data can be categorised by any user specified variable allowing for certain host-phases to be plotted and colour the datapoints by a specific variable. There is also functionality to export these figures if needed.

10.1 Organising .csv File

To get the full use out of the data explorer it is recommended that the .csv file contains the full apatite compositions, molar ratios, sample data and data on any host phases. A shortened example is shown below:

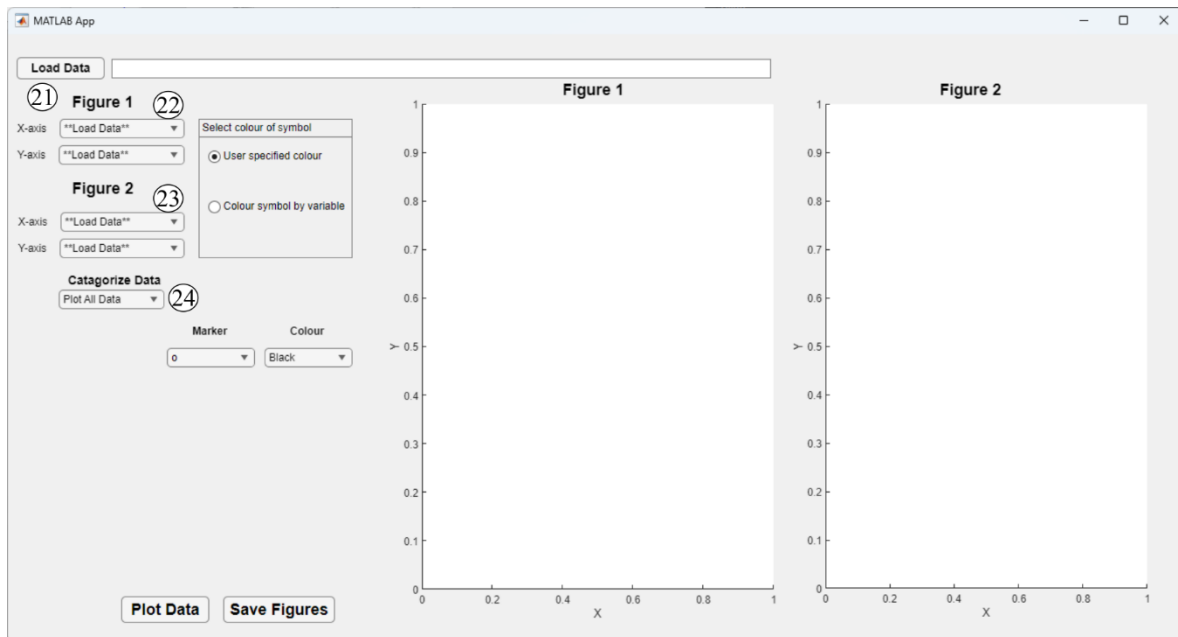
Sample	Phase	P2O5	CaO	MgO	Ce2O3	Cl	F	OH	Cl/OH	F/OH	F/Cl
Ap_1	Pyroxene										
Ap_2	Micro phenocryst										

The application determines which columns are categorical data by looking at the first row (below the headings). If the cell is text it is used as a category, if the cell contains a number it is used as a variable.

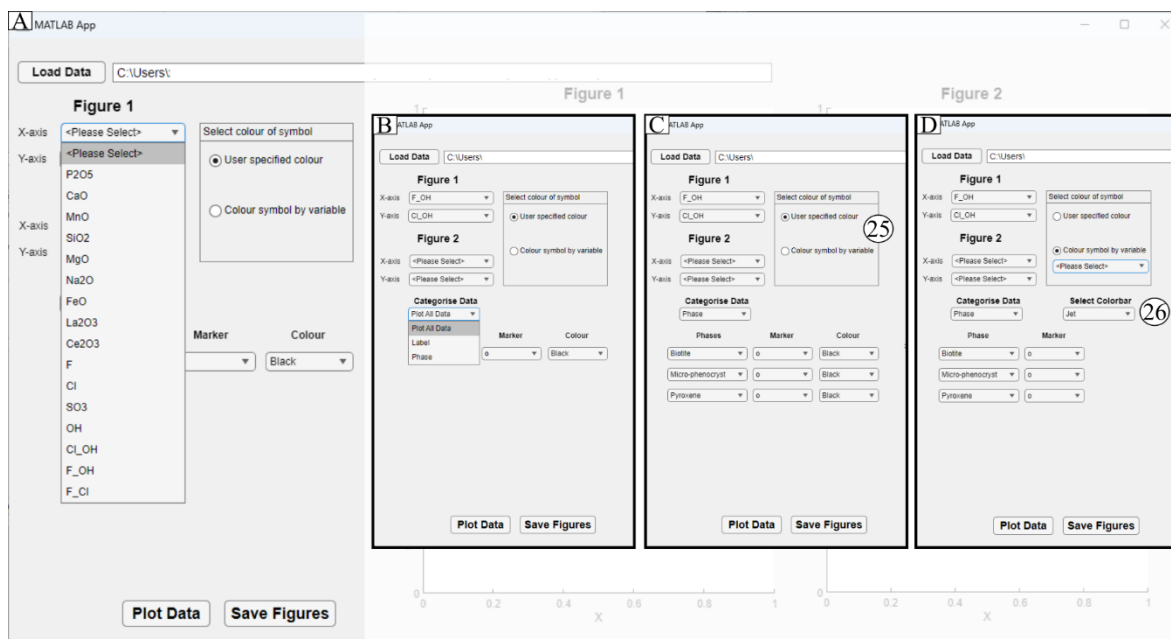
Ensure that all columns (excluding headings) are exclusively numbers or text. If the data in a single column is mixed the figure will not plot.

10.2 Using Data explorer

1. In the Multistart App click 'Open Data Explorer'. A new app will open (Figure 12)
2. Load data by clicking the Load Data button and navigating to a .csv file which contains the apatite data (Figure 12 [21]).
3. Once selected, the options for the X and Y axes for each of the two figures will be updated with the variable names for each column which contains numerical data (Figure 13A).
4. Click on the drop-down menu to select variables to plot (Figure 12 [22 & 23]). The X and Y variables for Figure 1 MUST be selected in order to plot a figure.



5. The '**Categorise Data**' drop down menu is set to '**Plot All Data**' by default (Figure 12 [24]). If the .csv file contains columns with string data (i.e. text) which can be used to categorise the data, these options will appear here. For instance, if there is a column with the name '**Phases**' and the column contains information on which phase the apatite inclusion was hosted in, the user can select this from the drop-down menu. For example, if the data has been collected from inclusions in pyroxenes and biotite as well as micro phenocrysts, 3 boxes will appear showing these phases alongside 3 boxes allowing the user to select a specific marker for each phase.
6. Once a category has been selected (Figure 13B & C), the user can choose the type of Marker to denote this feature.
7. Two options are available for selecting a colour for each feature. The user can specify one of the default MATLAB colours or the Markers colour can be determined by a third variable (Figure 13C [25]).
8. If '**User specified colour**' is selected drop-down boxes will appear and the user can select a colour.
9. If '**Colour symbol by variable**' is selected a drop-down box will appear where the user can select the variable they wish to use. A second drop-down box will appear where the user can select the colourmap they wish to use (Figure 13D [26]).
10. Click '**Plot Data**' to view the figures (Figure 13 [27]).
11. To save the figures, click '**Save Figures**' (Figure 13 [28]). A new figure will open including a legend and the user can edit the figure as they wish in the same fashion as the Multistart App (Section 3.6).



11 Warning messages in MATLAB App

Warning Code	Message	Why have I got this warning?	How do I fix this warning?
1	Warning 01: A custom TF file with this name already exists. Do you wish to overwrite it?	The user is trying to save a custom TF curve with the same name as a previously generated file within this folder.	Either overwrite the file if you wish to, or click 'No' and provide a new name for the TF curve.
2	Warning 02: This target file already exists. Would you like to overwrite it?	The user is trying to save a target curve with the same name as a file within the directory. This commonly occurs when you have loaded a previous run and wish to change the TF curve but forget to provide a new name for the file.	If you wish to overwrite the file, click 'Overwrite'. If you do not want to overwrite the file, click 'No'. You will need to either change the name of the target file or the model's name. If you are making a new target file to test different start parameters, it is recommended that you change the Model name.

3	Warning 03: The log file already exists! Do you want to overwrite it?	The user is trying to save a log file which already exists	If you wish to overwrite the file, click 'Overwrite'. If you do not want to overwrite the file, click 'No'. You must change the model's name to save a unique log file.
4	Warning 04: You will overwrite an existing MultiStart Output File! 10 'Do you wish to overwrite this file?	The user is about to run a multistart run, which will overwrite a previously created multistart file.	If you want to overwrite the multistart file, click 'Yes'. You will get another warning asking you to confirm the overwrite. If you do not wish to overwrite the file, click 'No' and give the model a new name or change the output folder. If you change the model's name, you must regenerate a target curve so that the file name matches the new model run. If you change the output folder, you must ensure your desired target file, log file and TF curve (if using one) are saved in that new folder.
5	Warning 05: This figure already exists in this file. Do you want to overwrite it?	The user is trying to save a figure with a file name that already exists	Either overwrite the file if you wish to, or click 'No'. You will need to resave the figures with different names.

12 Error messages

Error Code	Message	Why have I got this error?	How do I fix this error?
1	Error 01: You have not given this model run a name	The 'Model Run' field has been left blank.	You need to provide a name for the model run. This should be unique to distinguish between different runs. This will form part of the file names given you the outputs from the application.
2	Error 02: Data file not found; ensure that it is entered correctly	The 'Data file' field has been left blank, or the file does not exist	Ensure that a datafile has been selected and that it is a valid data file containing all the necessary fields
3	Error 03: No temperature option selected	The user has not defined how they would like to deal with temperature.	Use the Temperature drop-down menu to choose how to deal with temperature. Either set a constant temperature, load a predefined TF curve or generate a TF curve.

4	Error 04: TF curve not found	The user has selected the 'Load TF' curve option but has not specified a TF file, or the TF file does not exist.	Use the 'Load TF Curve' button to navigate a TF file. The TF file must have two columns only, with no titles for the columns. The first column must be the temperature in °C, and the second must be the melt fraction starting at one and decreasing.
5	Error 05: Temperature not set	The user has selected to input a constant temperature but has left the field blank.	Ensure the temperature value is set to an appropriate value for your magma type.
6	Error 06: Target file name not set	The target curve field has been left blank	Provide a name for the target file.
7	Error 07: Target file name is not valid	The file you are trying to load does not exist	If loading a previously generated target curve, select the appropriate log file and use the 'Load saved run' button. This will auto-populate this field with the target curve file name.
8	Error 08: No output file set	The user has not provided a name for the output folder where the model outputs will be saved.	Provide a name for the output file. This can be a new folder or an existing one. If you want to save to a current folder, it must be in the same folder as the data file, and you need to provide the file name and not the whole path.
9	Error 09: Parameter file not found	The user has tried to load a log file. However, the file cannot be found	Use the 'Load saved run' button to navigate to the _log file for the run you want to load.
10	Error 10: Set name for custom TF file	The user has chosen to generate their own TF file but has not provided a name for this file to save	Give the custom TF a name in the 'TF File Name' box.
11	Error 11: Error in MultiStart Bound. Check bounds to ensure they are set higher/lower than the initial start value.	The upper and lower bounds for the multistart are not greater than or less than the initial value. This error can also occur if the upper value is less than the lower value and vice versa.	Check the multistart upper and lower bounds to ensure that the upper bound is greater than the initial value and the lower bound is less than the initial value.

12	Error 12: Target file not found	The target file for the multistart run could not be found	Check the path in the error message. Check that the target file you wish to load is in the correct folder. For example, if the data file is saved in 'C:\users\model', the target file should be saved within the set output file within that folder.
13	Error 13: Target file not found	The user has clicked the 'Display multistart results' button or the 'Save Figures' button, and the app could not find the inputted target file.	Ensure that the name of the target file matches the name of the target file you wish to load and is saved in the output folder you have set.
14	Error 14: Target file not found	The user has loaded a previous run and clicked the 'Display multistart results' button or 'Save Figures' button, and the app could not find the inputted target file.	Ensure that the path to the desired target file is correct and the file exists in that folder.
15	Error 15: The .mat file containing the Multistart results could not be found. Ensure that the file path is correct and the .mat file is saved in the right place. "Path where the app tried to load the model from"	The app could not find the .mat file at the location of the user-specified	Check the path in the error message. Ensure that the file directory is set to the correct folder that contains the raw data file and that the 'Output File' field is set to the correct folder where the .mat file is saved.
16	Error 16: TF file not valid. Ensure the .csv file has two columns only. The first must be the temperature in degrees Celsius, and the second must be the melt fraction.	The TF file the user has tried to load contains more than two columns	Ensure that the TF file contains two columns only with no column titles. The first column must be the temperature in degrees Celsius, and the second must be the melt fraction.

17	Error 17: Log not valid. Ensure the file you are loading is a "_log.csv" file.'	The user is trying to load a log file which does not contain _log.csv in the file name and is, therefore, invalid.	Select a _log.csv file for the model run you wish to load.
18	Error 18: Some Variables were not found in the log file. Ensure the log file is valid.	The _log.csv file will be checked to ensure it contains all the necessary variables to auto-populate the required fields. If one or more of those variables does not exist, it will list them in the error message.	Check the log file to make sure the listed variables are present. You may need to generate a new target and log file with your desired parameters.
19	Error 19: File type not selected!	The user is trying to save the main figures but has not selected a file format.	Use the dropdown menu to select the type of file you wish to save the figures as.
20	Error 20 .mat file containing Multistart results not found. Ensure that the file path is correct and the .mat file is saved in the correct place. C\user\model...	The user is trying to save the main figures. However, the Multistart output file cannot be found.	Ensure that the path displayed in the error message is correct. Ensure the Directory and output file are set to where the Multistart .mat file is saved, and the 'Model run' field is set to the correct name for the model you wish to load.
21	Error 21: Invalid x and y limits. Inputs must be numeric values	The x and y limits supplied by the user are not numeric	You will need to resave the figures and enter valid x and y limits
22	Error 22: Invalid x and y limits. Ensure that the values for the upper limits are greater than the lower limits.	The values provided for the upper and lower limits are not valid. Either the upper value is less than the lower value, or the lower value is greater than the upper value.	You must resave the figures and enter valid x and y limits.

23	Error 23: Platform not supported	The platform you are trying to run the model on is not supported.	The model must be run on a PC or Mac.
24	Error 24: Invalid data file. The data file does not contain the necessary halogen data. Ensure that the file includes Cl/OH, F/OH and F/Cl data.	The file the user tries to load does not contain columns with the headings Cl/OH, F/OH and F/Cl.	Ensure the data file you are loading contains the halogen data and the columns are labelled with Cl/OH, F/OH and F/Cl.
25	Error 25: The Multistart file contains less than 20 entries and cannot be displayed	The Multistart file being loaded contains fewer than 20 entries.	If you want to display a multistart file with fewer than 20 start points, click 'Display Multistart Results'.
26	Error 26: Melt is oversaturated at the first step and cannot converge on a solution. Set Start F to 1	The initial conditions set have caused the melt to be oversaturated at the first step.	The model cannot run if the melt is oversaturated at the first step. Set F to a value closer to or at 1. Alternatively, alter the initial parameters so the melt is not oversaturated at the first step
27	Error 27: No successful Multistart runs. Change input parameters and rerun multistart	The multistart did not return any successful runs.	Change the upper and lower bounds used and rerun the multistart

28	<p>Error 28: Insufficient number of successful Multistart runs. Change input parameters and rerun multistart</p>	<p>There is an insufficient number of multistart runs to display.</p>	<p>There were fewer than two successful multistart runs, so the results cannot be displayed. Rerun the multistart with a higher number of start points or change the parameters of the multistart.</p>
29	<p>Error 29: No Multistart .mat file found</p>	<p>There is no Multistart .mat file in this folder</p>	<p>The multistart file you are trying to load is not in the output folder. This is either because a multistart hasn't been run with these conditions or the file has been moved or deleted.</p>
30	<p>Error 30: None of the local solvers returned a solution.</p>	<p>None of the multistart solvers converged to a successful solution</p>	<p>Change the multistart bounds so they are broader and rerun the multistart</p>

13 References

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