

# Phase stabilities with path-dependence

MJ Mayne, JF Moyen 14 February 2017 (for help contact mjmayne@outlook.com)



# Getting started

	Installation	2
	Concept	4
	Example1 – Simple	6
	Example2 – Phase extraction	10
	Example3 – Multi-path functionality	13
Referen	nce manual	
	Rcrust file management	15
	List of Parameters	16
	Useful functions	26
	Development	27
	Troubleshooting	28
	References	28

# **GETTING STARTED**

## Installation

Rcrust was developed using version 3.3.0 (2016-05-03) of R. Copyright © 2016 the R Foundation for Statistical Computing. To install Rcrust perform the following steps:

1. Copy the Rcrust folder to a location of your choice (preferably a root directory for example C:\ or D:\). The result should be similar to the picture below with all the Rcrust files contained in single directory for example D:\\Rcrust\

📕   🛃 📑 🖛 🛛 Rcrust			-	o x
File Home Share	View			~ 🕐
$\leftarrow$ $\rightarrow$ $\checkmark$ $\uparrow$ $\square$ $\rightarrow$ This	s PC → LENOVO (D:) → Rcrust ←①	✓ ひ Search Rcru	st	م
A Quick access	Name	Date modified Type	Size	
OpeDrive	📙 bin	03 May 2016 5:08 File folder		
Chebiwe	📙 help	03 May 2016 4:50 File folder		
💻 This PC	License	27 Apr 2016 10:03 File folder		
E. Desktop	Projects	03 May 2016 4:00 File folder		
Documents	📙 R installs 🗲 📿	03 May 2016 5:04 File folder		
🚽 Downloads 🗸	README	15 Sep 2015 4:24 PM File		4 KB
6 items 1 item selected				

Figure 1 - Rcrust file structure located in the root directory D:\\Rcrust\

Install a working version of R on your system (at least version 3.3.0). The latest version of R used in the development of Rcrust is located in the folder "R installs" for your convenience.
 Warning: Rcrust requires the 64 bit version of R. When installing R please ensure "64-bit Files" is ticked.

🔂 Setup - R for Windows 3.3.0	_		×
Select Components Which components should be installed?			R
Select the components you want to install; dear the components install. Click Next when you are ready to continue.	you do not	t want to	
User installation		、 、	-
		66,7 M	3
32-bit Files		43,8 M	3
64-bit Files		44,4 M	3
Message translations		7,3 ME	3
Current selection requires at least 163,0 MB of disk space.			
< <u>B</u> ack	<u>l</u> ext >	Car	ncel

Figure 2 - R installation instruction ensuring at least "64-bit Files" is ticked

\*Alternatively newer versions of R (which may not be compatible with Rcrust) can be downloaded from <u>http://www.r-project.org/</u> or for windows can be found directly at <u>http://cran.r-project.org/bin/windows/base/</u>

3. Open the folder called bin in the Rcrust folder.



Figure 3 – Rcrust file (circled in red) within bin folder. The Rcrust file location here is D:\\Rcrust\bin\Rcrust.RData

- 4. Copy the Rcrust file found in the bin folder (~/Rcrust/bin/Rcrust.RData). This can be done by right clicking on the file (circled in red above) and selecting "Copy" or by selecting the file and pressing "Ctrl"+"c".
- 5. Paste the Rcrust file as a **shortcut** on the Desktop. This can be done by right clicking on the Desktop and selecting "**Paste shortcut**".



Figure 4 – Paste shortcut option selected for Rcrust file

- 6. Rename this file to "Rcrust". Double click on this shortcut to open Rcrust.
- 7. Rerust requires the R package called "shiny", If this is not installed on your computer when you open Rerust, Rerust will try to install it (this requires an internet connection). Follow the prompts to complete installation of the package (it may ask you if you wish to create a personal library choose yes). Alternatively, shiny can be downloaded here: <a href="http://shiny.rstudio.com/">http://shiny.rstudio.com/</a>.

Each new project will be automatically saved in the "Projects" folder along with its associated inputs and outputs. To load a previously saved project simply double click the "xxx.RData" file in the associated project folder or open Rcrust from the desktop shortcut and load the project via the Rcrust GUI.

# Concept

Rcrust is an R program aimed at modelling with path dependence. The program functions by calculating a number of points in P-T-X space where a bulk composition is passed between points. This creates path dependence as points within the path rely on the outcomes of previous points for their calculation. The bulk composition can be altered at each point by phase manipulations consisting of phase additions and/or phase extractions.

Rcrust manages calculations by splitting the full thermodynamic system (FS) into 3 subsystems: The reactive subsystem (RS) which contains the phases in thermodynamic equilibrium; The addition subsystem (AS) where phases are waiting to be added to the reactive subsystem; and the extract subsystem (ES) where phases extracted from the reactive subsystem are stored. The reactive subsystem is in thermodynamic equilibrium with the P-T-X conditions of each point and is re-equilibrated after each P-T-X change. The addition and extract subsystems are in thermodynamic isolation from other subsystems and from the P-T-X conditions of each point.



Figure 5 - Relationships between systems (left) and flow chart (right) illustrating the Rcrust program structure for a single path. The user inputs the calculation's resolution, starting bulk composition, P-T path and phase manipulation settings. Each step in a path consists of two runs and an output. The first run is shown in a solid line, the second run in a dashed line and the outputs in a dotted line. Circles show the system or subsystem involved in each step as AS (addition subsystem), ES (extract subsystem), FS (full system) or RS (reactive subsystem). Arrows show interactions between systems. From (Mayne et al. 2016)

Parameters for calculations are accessible to the user via the Rcrust Graphical User Interface (GUI). This GUI writes data to a text file which is then input to the program thus allowing the user to edit the file 'behind' the GUI as well as save inputs for re-use. The code files are extensively commented, and described in this document. The calculations routines are defined in several files, written in a modular way that should allow easy addition of features if required. For example, the Phase Extraction routine has been modified to suit the needs of magma extraction where additional capabilities allow melt extraction to leave a set melt retention amount behind.



Figure 6 - Flow chart of the magma extraction routine. Grey hexagon shaped boxes are decision points. Coding variables are in italics. The for phase loop (dotted line) is repeated until each phase tagged for extraction has been considered. If Retention mode is active melt is considered last so that other phases extracted are accounted for in its calculation. From (Mayne et al. 2016)

Rcrust results should easily be loaded into GCDkit and examined from there.

It is important to remember a few things:

- Rcrust is in development. It is not mature software. It is very unstable at the best of times, and very unforgiving in terms of improperly formatted inputs, etc. When Rcrust fails, it will try to generate some human-readable error messages: read them! It may well give you hints at things you can correct in your inputs.
- Most of the errors you will see are related to incorrect input (files with incorrect number of lines etc.); or to exotic phases being produced by meenum.

Rcrust calls a set of binary files containing the thermodynamic equations thus relying on published databases (Holland and Powell typically). The output will never be better than the underlying thermodynamic model. Since we focus on melting, we are tied to the capacities (and limitations) of the melt models. For example, melt(HP) does not include Titanium therefore its use in a system containing Ti can over/under estimate melt abundance.

# **Examples**

Below are 3 example simulations to get you started using Rcrust. All you need to do to complete the examples is to perform the actions written in bold numbered text. Explanations of what these actions achieve are given between steps.

Example1 - Simple

#### Follow the bold numbered steps

To begin the first example open Rcrust via the desktop shortcut.

#### 1. Double click the Rcrust desktop shortcut

This will launch the R console and an empty Rcrust Graphical User Interface (GUI) in your default web browser. The "**Working File**" (circled in red) shows you which file is currently being worked on and the "**Projects Directory**" (circled in green) shows you where the projects folder is located. The Rcrust toolbar (in grey) contains buttons for file management.

Projects Directory D:/Rcrust/Projects Working File  Rcrust Save Load Run Clear Close	Projects Directory           Working File
Input Parameters Phase Manipulations Modelling Options Outputs	Rcrust Toolbar
	R Rou (2-br) - > Fe fat Yew Mix Bedages Windows Help Br Ch Ba Ba - Ba - Ba
Pressure and Temperature Number of PT definitions	R Version 3.2.4 Revised (2016-03-16 r70336) "Very Secure Dishes" Copyright (c) 2016 The R Foundation for Statistical Computing Platform: 138-ev6-inny024/3386 (2-2-bit) R is free software and comes with ABSOLUTELY NO WARBANTY. You are veloceme to redistribute it under certain conditions. Type "license()' or distribution details. Natural language sup
Bulk Composition Major elements	R is a collaborative pr Type 'dontributican's and the second sec
Number of bulk definitions	[Previously saved workspace restored] Listening on http://127.0.0.1:6453
Import definitions from file	

Figure 7 -Rcrust GUI and R Console (blue). Highlighted are the positions of the Projects Directory (green), Working File (red) and Rcrust toolbar (black).

# 2. Type "Example1" into the text box on the right of Working File and then click the Load button from the Rcrust toolbar

The data previously saved in the "Example1" file is now loaded into R and previously saved input parameters are loaded into the Rcrust GUI. To ensure that we do not overwrite any data lets rename the Working File.

# **3.** Rename Example1 by typing "Example\_simple" into the Working File textbox then click the Save button from the Rcrust toolbar

This will save the current Rcrust GUI inputs into a new file named "Example\_simple". The Rcrust GUI should now look similar to Figure 8.

Size	1	Working File Example1				Directory C:/Ro	Project			
Size       Input Parameters       Phase Manipulations       Modeling Options       Outputs         Size       Imput Parameters       Phase Manipulations       Modeling Options       Outputs         Size       Imput Parameters       Phase Manipulations       Modeling Options       Outputs         Imput Parameters       Phase Manipulations       Modeling Options       Outputs         Imput Parameters       Y       Imput Parameters       Imput Parameters         Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters         Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters         Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters         Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters         Imput Parameters       Imput Parameters       Imput Parameters       Imput Parameters <th>onsole Close</th> <th>Clear</th> <th>Run</th> <th>Load</th> <th>Save</th> <th></th> <th>st</th> <th>Rcrus</th> <th></th> <th></th>	onsole Close	Clear	Run	Load	Save		st	Rcrus		
Number of Programmeters       Phase Manipulations       Modelling Options       Outputs         Size      x      x					1.txt	1/Inputs/Examp	rojects/Examp	Loaded C:/Rcrust/Pr		
Size       x       y         X       y         4       3         Pressure and Temperature       Pressure and Temperature         Number of PT definitions         1         From       To         Pressure (kbar)         (11)         (4:3)         7.y_i         670+x_i'20         Bulk Composition         Number of Component Transformations         Major elements         NA20 MGO AL203 SI02 K20 CA0 TI02 FE0 02 H20         Number of bulk definitions			Outputs	otions	de <b>lli</b> ng Op	ipu <b>l</b> ations I	Phase M	Input Parameters		
SIZE       X       Y         4       3         Pressure and Temperature          Number of PT definitions       1         From       To       Pressure (kbar)         Temperature       (11)       (4.3)         Bulk Composition          Number of Component Transformations         Major elements         NA2O MGO AL203 SIO2 K20 CA0 TIO2 FE0 02 H20         Number of bulk definitions								Size	Sizo	
Pressure and Temperature          Number of PT definitions       1         From       To       Pressure (kbar)         Temperature       (1:1)       (4:3)         Bulk Composition          Number of Component Transformations         Major elements         NA2O MGO AL203 SIO2 K20 CA0 TIO2 FED 02 H20         Number of bulk definitions							Y	x		
Pressure and Temperature          Number of PT definitions       1         1       From       To       Pressure (kbar)       Temperature (C)         {11}       (4:3)       7-y_i       670+x_i'20         Bulk Composition        Number of Component Transformations         Major elements       NA20 MGO AL203 \$J02 K20 CA0 T[02 FE0 02 H20         Number of bulk definitions       Number of bulk definitions							3	4		
Pressure and Temperature          Number of PT definitions       1         From       To       Pressure (kbar)       Temperature (C)         [1]       [4:3]       7-y_i       670+y_i*20         Bulk Composition        Number of Component Transformations         Major elements       NA20 MGO AL203 SI02 K20 CA0 TI02 FE0 02 H20         Number of bulk definitions										
Pressure and Temperature       1         From       To       Pressure (kbar)         [1]       [4:3]       7-y_i         [1]       [4:3]       7-y_i         [1]       [4:3]       7-y_i         Bulk Composition          Number of Component Transformations         Major elements         NA2O MGO AL203 SI02 K20 CA0 TI02 FE0 02 H20         Number of bulk definitions							mperature	Pressure and Ter		
Temperature       To       Pressure (kbar)       Temperature (C)         {1:1}       {4:3}       7-y_i       670+x_i'20         Bulk Composition       Mumber of Component Transformations       Major elements         NA2O MGO AL203 SJ02 K20 CA0 TI02 FE0 02 H20       Number of bulk definitions		Dressure and								
From       To       Pressure (kbar)       Temperature (C)         (1;1)       (4;3)       7-y_i       670+x_i'20         Bulk Composition        Number of Component Transformations         Major elements       NA20 MGO AL203 SI02 K20 CA0 TI02 FE0 02 H20         Number of bulk definitions			Tomporeture							
Bulk Composition Number of Component Transformations Major elements NA20 MG0 AL203 SI02 K20 CA0 TI02 FE0 02 H20 Number of bulk definitions		670+x i*20				Pressure (I	To	From	remperature	
Bulk Composition Number of Component Transformations Major elements NA20 MG0 AL203 SI02 K20 CA0 TI02 FE0 02 H20 Number of bulk definitions		0+X_120	011				[4,0]	1.17		
Bulk Composition Number of Component Transformations Major elements NA20 MG0 AL203 SI02 K20 CA0 TI02 FE0 02 H20 Number of bulk definitions										
Bulk Composition Number of Component Transformations Major elements NA20 MGO AL203 SI02 K20 CA0 TI02 FE0 02 H20 Number of bulk definitions							·	Bulk Composition		
Bulk Composition						rmations	ponent Trans	Number of Com		
Bulk Composition Major elements NA20 MGO AL203 Sl02 K20 CA0 TI02 FE0 02 H20 Number of bulk definitions										
Bulk Composition Number of bulk definitions		Major elements								
Composition Number of bulk definitions		Bulk								
		Number of bulk definitions								
1								1		
From To NA2O,MGO,AL2O3,SIO2,K2O,CAO,TIO2,FEO,O2,H2O,ma	nass	,FEO,O2,H	AO, TIO2,	02,K2O,C	L2O3,SIC	NA2O,MGC	То	From		
{1;1} {4;3} 1.82,3,28,20,45,56,97,4,09,1,56,1,05,8,50,16,1,96,100	0	5,0.16,1.96	6,1.05,8.5	,4.09,1.5	45,56.97	1.82,3.28	{4;3}	{1;1}		

Figure 8 - Rcrust GUI with Example1 (Example\_simple) parameters loaded. The GUI consists of a number of tabs. The Input Parameters tab sets the size, P-T conditions and bulk composition (X) of the simulation.

This example calculates the phases encountered at points in P-T-X space. Input parameters are grouped into collapsible panels:

• Size Panel

The **Size** panel sets the number of points in the simulation (here 4 points in the **X** direction multiplied by 3 in the **Y** direction). Points in the simulation space are identified by **tuples** written as  $\{x_i, y_i\}$  where i denotes the current point.



Figure 9 – Simulation space with point coordinates defined by tuples {x\_i ; y\_i}

• Pressure and Temperature Panel

Parameters in the simulation space are filled by a number of definitions. Each unique definition is applied over a range between the tuples **From** {  $x_a$ ;  $y_a$  } and **To** {  $x_b$ ;  $y_b$  } where a and b denote the start and end points of a rectangular range. Each definition sets its attributes as constants or as functions of the point's position. **X** and **Y** positions of points are accessed by the variables  $x_i$  and  $y_i$  respectively. In the **Pressure and Temperature Panel** we set the Pressure in kilobars and

Temperature in degrees Celsius for each point. In this example **Pressure** decreases along the y-axis by 1 kbar per point (7-y\_i) and **Temperature** increases along the x-axis by 20 °C per point (670+x\_i\*20).

• Bulk Composition Panel

The **bulk composition** of the system is made up of a number of major elements expressed as wt.% elemental oxides. For this simple example we define the bulk composition to be constant across the full P-T space, and we give it the value of the average amphibolite-facies pelite composition considered in (Mayne et al. 2016).

	Na <sub>2</sub> O	MgO	Al <sub>2</sub> O <sub>3</sub>	SiO <sub>2</sub>	K <sub>2</sub> O	CaO	TiO <sub>2</sub>	FeO	<b>O</b> 2	H <sub>2</sub> O
wt.%	1.82	3.28	20.45	56.97	4.09	1.56	1.05	8.5	0.16	1.96
Table 1 – Average amphibolite facies pelite composition considered in (Mayne et al. 2016).										

To get started let's run a reconnaissance simulation:

#### 4. Click the Run button from the Rcrust toolbar

This will save inputs in the Rcrust GUI and launch the calculation procedure into the R console. Navigate to the R console now. The R console should now have a few lines of text in it (like the figure below): If your simulation successfully initialized like the one below then we are ready to start the calculation. If your console failed to initialize the program try reloading the original "Example1" file by closing Rcrust then starting from step 1 again, if problems persist try reinstalling Rcrust or report the problem to the developers (mjmayne@outlook.com).

🥂 RGui (32-bit)	-		$\times$
<u>F</u> ile <u>E</u> dit <u>V</u> iew <u>M</u> isc <u>P</u> ackages <u>W</u> indows <u>H</u> elp			
2 4 I I I I I I I I I I I I I I I I I I			
R Console			× (
Type 'demo()' for some demos, 'help()' for on-line help, or 'help.start()' for an HTML browser interface to help. Type 'q()' to quit R.			
[Previously saved workspace restored]			
Listening on http://127.0.0.1:7418			
Initializing bulk composition			
Bulk composition defined from inputs P-T-X space under investigation with $x = 4$ and $y = 3Creating bulk compositions from definitions in configurationDone with bulk composition preparation$	file		
Creating meemum build file Created meemum build file as D:/Rcrust/bin/parse_meem.dat			
Initializing PT conditions Calculating PT conditions from inputs Done with PT conditions			
No phase addition. Done with phase addition options			
No phase extraction. Done with phase extraction options			
Done with dependence determination			
Initiation succesful:			
Please read the above lines and make sure this is what you Choose "n" to abort or press [enter] to continue	u wante	ed.	
			~
<	_		>

Figure 10 - The Rcrust calculation is launched into the R Console which tracks the calculation progress and is currently waiting for a response to continue or to abort.

5. Click anywhere in the R console to activate it then press [enter] to continue

The calculation will run for 12 points :4 in the X direction by 3 in the Y direction. The results will automatically be saved to file and you will be prompted to select outputs.

# 6. Once the calculation is complete, navigate back to the Rcrust GUI and Select the Outputs tab

Here we see a compilation data file for the points in our simulation. To compare points, click the "Select Output" drop down and choose "Grid".

#### 7. Choose "Grid" under "Select Output"

Grid allows easy comparisons between points for example choose:

- Select Output = Grid
  - Variable = wt% and Melt\_rs

#### 8. Choose Variable="wt%" and "Melt\_rs"

The output should now match Figure 11. This shows us the amount of melt in the Reactive Subsystem (RS) over our point selection in P-T-X space. Remember we set temperature to increase along the x-axis and pressure to decrease along the y-axis. With that in mind, we see that the solidus (boundary between liquid and solid) at lower pressures is crossed by lower temperatures (this is a good illustration of the pressure dependence of melting).

For further outputs you can deal directly with the data in the R console (hint: you can plot data directly into GCDkit). To access the data in R console, click the "Console" button on the Rcrust toolbar to launch a browser access. To return to the Rgui at any point type "c" then press [enter].

/lelt	t_rs wt	% on (	(X,Y) gi	rid	
	V1	V2	<b>V</b> 3	V4	Figure 11 – Grid output Data for Example_sin
1	0.00	0.00	12.59	14.91	showing weight percentage of melt in the reac
2	0.00	8.74	10.21	11.26	subsystem for the F-1-X points selected
3	0.00	8.20	9.07	10.32	

To view a graphical output of this data toggle the "View" selection to "Plot". This will plot a filled contour graph of the selected data which can be saved directly as a .ps file through the "Save To File" button at the bottom of the selection panel.

# 9. Toggle the "View" selection from "Data" to "Plot" and choose "Bottom Axis" as "Temperature", "Left Axis" as "Pressure"



#### Example2 – Phase extraction

Phase extractions can remove phases from the reactive subsystem. This is used to simulate scenarios such as melt loss or fractional crystallization.



**Figure 13 – Example of melt extraction along a P-T-X path from** (Mayne et al. 2016): Weight percentage of phases verses temperature in degrees Celsius for a fixed pressure of 12 kbar. Starting composition taken as an average amphibolite facies pelite (Table 1). Melt is extracted whenever a 7 vol.% threshold is met.

Let's perform melt extraction along a path in the P-T-X space explored by Example1.

1. Load Example2 by opening Rcrust, typing 'Example2' in working file and clicking "Load"

To ensure that we do not overwrite any data lets rename the Working File.

2. Rename the file by typing "Example\_extract" into Working File then click the Save button from the Rcrust toolbar

This will save the current Rcrust GUI inputs into a new file named "Example\_extract". The Rcrust GUI should now look like the images below:

	Projects	Directory C:/R	crust/Project	ts	Working File Example2			Projects Dire	ctory C:/	C:/Rcrust/Projects			Working File Example2			
Rcrust			Save	Load	Run Clear	Run Clear Console Close		Rcru	st		Save	Load	Ru	n Clear	Console	
<pre>le saved to C:/Rcrust/Projects/Example2/Inputs/Example2.txt</pre>							Loaded C:/Rcrust/Projects/Example2/Inputs/Example2.txt									
nput Parame	ters Phase Ma	nipulations	Modelling O	ptions	Outputs			Input Parameters	Phase Manipul	ations	Modelling	Options	Outp	uts		
Size X	Y							Phase Addition	 							
								Perform Phase	e Addition?							
Pressure and Number of P	Temperature							Phase Extraction	-							
1								Perform Phase	e Extraction?							
From	То	Pressure	(kbar)		Temperature	(C)		Phases for extra	action							
{1;1}	{25;1}	12			760+x_i*5			Melt								
								Number of extra	action definitions							
Bulk Compos	ition							1								
Number of C	omponent Trans	ormations						From	То	Conditio	n					
								{1:1}	{25:1}	Melt,>=	,7,wt%					
Major eleme	nts							Melt								
NA2O MG	0 AL203 SI02	(20 CAO T <b>I</b> O2	2 FEO 02	H2O				100%								
Number of b	ulk definitions															
2																
From	То	NA2O,MG	0,AL203,S	O2,K2O,C	CAO, TIO2, FEO, O2,	H2O,mass										
{1;1}	{1;1}	1.82,3.2	8,20.45,56.9	7,4.09,1.5	56,1.05,8.5,0.155,1	.96,100										
From	То	NA2O,MG	0,AL203,S	Ю2,K2O,C	CAO, TIO2, FEO, O2,	H2O,mass										
	(05.4)															



This example calculates an open system dependent path in P-T-X space. The bulk composition of the Reactive Subsystem is altered by phase manipulations encountered along the path. Phase Manipulations are grouped into collapsible panels:

Phase Addition

Phases such as intruding fluids, segregated melts or residual crystals can be incorporated into the reactive subsystem. These additions are defined by the major elemental oxides chosen in "Bulk composition".

• Phase Extraction

Phases in the reactive subsystem can be extracted when set conditions are met. These conditions are defined as logical arguments such as "TRUE"/"FALSE" to extract for every point/no points respectively. Alternatively a logical argument can be built of the form "phase,operand,value,unit" where phase = name of the phase/solution model, operand = (<,<=,==,>=,>,!=), value = a number and unit = the phase property to test. In this example we want to trigger extraction whenever a melt threshold is reached so our conditional argument is "Melt,>=,7,wt%". \*note that each argument in the condition is separated by a comma.

When the condition is met phase extraction is triggered on the reactive subsystem. For each phase listed in **Phases for Extraction** we need to define the amount of the phase to extract. This can be a numeric value (interpreted as grams relative to the starting mass in grams defined in the Bulk Composition Panel), or a percentage of the current value. In this example we extract all melt (100%).

Phase Extrac	ction		
Perform F	hase Extraction?		
Phases for e	extraction		
Melt			
Number of e	extraction definition	ns	
1			
From	То	Condition	
{1;1}	{25;1}	Melt,>=,7,wt%	
Melt			
100%			

Figure 15 - Phase extraction definition for Example\_extract

To save you time we have pre-run this calculation so you can directly view the results by selecting the **Outputs** tab.

#### 3. Select the Outputs tab in the Rcrust GUI

A custom output selection is available for viewing phase abundances along a path.

#### 4. Choose "Phase Abundance Along Path" under "Select Output"

Here you can select which axis the path traverses (axis), which path you wish to consider (path), select the (Start Point) and (End Point) of the path and add a label for the column names.

#### 5. Set "End Point" as 25

The output should now match Figure 16.

	•	R	cru	st

Projects Directory	C:/Rcrust/Projects	Example_extract	Save		Load	Run	
				Clear	C	onsole	Close
Recults cauged to Co./Remus	+/Projects/Example a	tract/Evample.ev	tract PData				

Calculation complete, Results saved to C:/Rcrust/Projects/Example\_extract/Example\_extract.RData Select outputs throught the 'Outputs' tab

Input Parameters Phase Manipulat	ons Modeling Options	Outpu	its												
Phase Aliases	Phase adundar	nce vs Te	emperatu	ire(C) fo	or {1;1}	to {25;1	}								
		765	770	775	780	785	790	795	800	805	810	815	820	825	830
	Gt_rs	19.13	19.14	19.49	21.17	21,21	22.22	23,29	24.11	24,28	25.54	26,51	27,48	27.67	27.72
Select Output	Melt_rs	3.92	4.35	0.00	5.63	5.92	6.31	0.00	0.33	0.41	1.00	1.48	1.97	2.15	2.21
Phase Abundance Along Path 🔹	Mica_rs	26.89	26.27	12.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
View	Bio_rs	8,68	8.67	9,59	8,59	8.45	7.22	5.77	4.81	4.56	2,93	1.56	0,39	0.15	0.00
Data	Fsp_rs	17.69	17.81	13.58	9.05	8.92	8.42	8.14	7.57	7.66	7.12	7.14	6.47	6.35	6.70
Axis	llm_rs	2.35	2.35	2.23	2.31	2.32	2.39	2.48	2.53	2.55	2.66	2.78	2.88	2.90	2.91
×	ky_rs	1.54	1.72	6.73	11,00	10,93	10.76	10,48	10.37	10,31	10.00	9,67	9,48	9.44	9.37
	q_rs	19.81	19.67	17.32	14.45	14.37	13.95	13.45	13.12	13.03	12.47	11.98	11.54	11.45	11.38
Path	Mic_rs	0.00	0.00	8.81	18.18	18.25	19.11	19.99	20.77	20.81	21.89	22.47	23.39	23.49	23.32
1 •	ru_rs	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Start Point	Bulk_rs	100.00	100.00	90.38	90.38	90.38	90.38	83.60	83.60	83.60	83.60	83.60	83.60	83.60	83.60
1 *	Melt_es	0.00	0.00	9.62	0.00	0.00	0.00	6.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Bulk_es	0.00	0.00	9.62	0.00	0.00	0.00	6.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00
End Point	Melt_es_cumul	0.00	0.00	9.62	9.62	9.62	9.62	16.40	16.40	16.40	16.40	16.40	16,40	16.40	16.40
25 *	Bulk_es_cumul	0.00	0.00	9.62	9.62	9.62	9.62	16.40	16.40	16.40	16.40	16.40	16.40	16.40	16.40
Column Names															
Temperature(C) •															
File type															
.csv 👻															
Save To File															

Figure 16 – Phase Abundance Along Path output for Example\_extract showing mass of each phase in the full system (FS) across the P-T-X points selected.

This output highlights a few key features of the phase extraction function:

• The first melt extraction event extracts more than 7 wt% melt (relative to the full system)(red box) even though the melt extraction threshold was set to be 7 wt%

Reason -> Evaluations are only performed at each point thus if the resolution (number of points) is low then large changes can occur between each point. (the previous point (orange box) had less than 7 wt% melt so did not exceed the melt extraction threshold.

• Subsequent melt extraction events may appear less than the melt extraction threshold (green boxes)

Reason -> The melt extraction threshold is evaluated relative to the Reactive Subsystem (which itself is shrinking due to melt extraction events) thus equivalent proportions of melt equate to different proportions when compared to the full system (FS).

Further points to note about phase extraction are:

- Extracts are not thermodynamically re-equilibrated to the reactive subsystem or the P-T conditions and can be compilations of multiple phases in solid solution.
- The reactive subsystem is re-equilibrated after each extract so may produce new instances of a phase that were extracted.

#### Example3 - Multi-path functionality

Multiple paths can be compiled in P-T-X space to produce path-dependent P-T mode diagrams. In these diagrams a plane in P-T space is filled with points originating from dependent paths.



Let's create a path-dependent P-T mode diagram by decompressing off of the path investigated in Example2.

1. Load Example3 by opening Rcrust, typing 'Example3' in working file and clicking "Load"

To ensure that we do not overwrite any data lets rename the Working File.

2. Rename the file by typing "Example\_multi" into Working File then click the Save button from the Rcrust toolbar

This will save the current Rcrust GUI inputs into a new file named "Example\_multi". The Rcrust GUI should now look like Figure 18.

	Projects	D/Rcrust/Projects	ctory D/Rcrust/Projects Working File Example3 Projects Directory D/Rcrust/Projects		D:/Rerust/Projects	acts Working File Example3											
Rc	rust		Save	Load	Run C	lear	Close	RCrL	JST				Save	Load	Run	Clear	Clos
culation con lect output:	mplete, Results s s throught the 'O	aved to D:/Rcrust/Projects/Ex utputs' tab	cample3/Ex	cample3.RE	Dota			Calculation compl Select outputs t	ete, R hrough	esults say t the 'Out	ed to D:/ puts' tab	Rcrust/Projects/I	xample3/F	xample3.P	llata		
Input Parame	aters Phase Ma	anipulations Modelling Optic	xns O	ulputs				Input Parameter	rs	Phase Mar	nipulations	Modelling Opt	ions C	lutputs			
Size								Phase Addition									
x	Y							Perform Pha	ase Ado	dition?							
19	1	1															
								Phase Extractic	m								
Pressure an	d Temperature							Perform Pha	ase Ext	raction?							
Number of I	PT definitions							Phases for ext	traction	n							
1								melt(HP)									
From	То	Pressure (kbar)		Tempera	ture (C)			Number of ext	raction	definition	ns						
{1;1}	{19;11}	12-(y_i-1)*0.3		660+(x	_i-1)*10			1									
								From	То		Condi	ition					
								1,1	1	9,11	melt	(HP),>=,7,wt%					
Bulk Compo	sition	formations						melt(HP)									
	somponent mana							retain(1,wt%)	i i								
	1213																
NA2D MC		K20 CA0 TIO2 EEO O2 H20	<b>.</b>														
10420 1010	AL200 0102 1	120 040 1102 1100 02 1120															
Number of I	oulk definitions																
3																	
From	То	NA20,MGO,AL203,SI02,	K2O,CAC	,TIO2,FEC	D,O2,H2O,m	<b>ass</b>											
{1:1}	{1:1}	1.82,3.28,20.45,56.97,4	.09,1.56,1	.05,8.5,0.1	155, 1.96, 100												
From	То	NA20,MGO,AL203,SI02,	K20,CAC	TIO2,FE	0,02,H2O,m	ass											
{2;1}	{19;1}	rs{x_i-1;y_i}															
From	То	NA20,MGO,AL203,SI02,	K20,CAC	,TIO2,FEC	0,02,H2O,m	ass											
1,2	19,11	rs{x_i;y_i-1}															
Import de	finitions from file																
- mport de																	

Figure 18 - Rcrust GUI inputs for Example\_multi

This example creates a composite path-dependent P-T mode diagram. It does this by first calculating an open system isobaric heating path at 12 kbar (IBH12) and then calculating a number of isothermal decompression paths that each originate from a point on IBH12. Points along IBH12 are each dependent on the reactive subsystem of the point one to the left of itself on the x-axis. Points along decompression paths are each dependent on the point one above itself on the y-axis. Melt loss is defined to occur whenever a 7 wt.% melt threshold is met and melt is extracted until 1 wt.% melt is left behind (this is achieved using the "retain(amount,unit)" function).



Figure 19 - Grid output for Example\_multi showing weight percent of melt in the reactive subsystem (RS)

# **REFERENCE MANUAL**

# **Rcrust File Management**

The top line of the Rcrust GUI hosts a toolbar of file management buttons. User inputs are saved in a text document (**Working File**) which is located in the Projects folder of Rcrust (**Projects Directory**). This file is written, read or run in Rcrust by the **Save**, **Load** and **Run** buttons.

						Projects
Projects Directory D:/Rcrust/Projects		orking Fil	e Examp	ole1		Working File
Rcrust	Save	Load	Run	Clear	Close	
Loaded D:/Rcrust/Projects/Example1/Inputs/Example1.txt			-		-	Rcrust Toolbar
						Status

#### Save

Saves the **Working File's** inputs and calculation results. Each working file is assigned its own project folder in the **Projects Directory**. Parameters currently in the Rcrust GUI are saved to the Inputs folder as a text document. Additional parameters can be passed to Rcrust by placing them in the text document after the line (# Additional Parameters). Calculation results are saved as an R workspace in the project folder.

#### Load

Loads the **Working File's** inputs and calculation results. Reads the working file from the inputs folder and loads its options in the Rcrust GUI. Replaces the current workspace with that of the **Working File's**.

#### Run

Saves the current Rcrust GUI inputs and runs the Rcrust calculation according to these parameters. Follow prompts in the R console to calculate the results. Once the results are complete you will be prompted to select outputs through the Rcrust GUI. Outputs written to file are saved in the Ouputs folder of the project Advanced users can access the results directly in the R console by pressing [esc] to activate the console (this is helpful for loading data into GCDkit). To relaunch the Rcrust GUI type 'runApp()' then press [Enter]

#### Clear

Clears current values in the Rcrust GUI

#### Console

Launches a browser in the R console giving you direct access to the coding environment and all calculated data

#### Close

Closes the Rcrust GUI. To relaunch the Rcrust GUI type 'runApp()' then press [Enter]

# **List of Parameters**

User inputs are listed here in a systematic fashion for clarity. The parameter name (the name that appears in the Rcrust GUI) is listed first followed by the variable name (the name of the variable accessible in the R console). The data type required for the parameter is listed in the second box. The third box contains possible values for the parameter and identifies any default value. Below this is a description as to what the parameter controls.



#### **Input Parameters**

#### Tuple definitions

From {pt_from_#}	Tuple	${1;1} \le pt_from_# <= {x_n;y_n}$
The beginning of the definition se	lection	

To {pt_to_#}	Tuple	pt_from_#<=pt_to_#<={x_n;y_n}
The end of the definition selectio	n	

#### Size

Specify here the size of the simulation (resolution) you want to calculate: how many points in the X and Y directions.



#### **User Interface**

X	Numeric	1< x_n
{x_n}		
The total number of points in the	X direction	

Y {y_n}	Numeric	1< y_n
The total number of points in the	Y direction	

# Pressure and Temperature

ı	Number of P	T definitions			
	1				
F	From	То	Pressure (kbar)	Temperature (C)	
	{1;1}	{19;11}	12-(y_i-1)*0.3	660+(x_i-1)*10	

# **User Interface**

Number of PT definitions {n pt def}	Numeric	1< n_pt_def
The number of definitions to use t	for assigning pressure and temperat	ure values

Pressure (kbar)	Numeric/Expression					
{pressure_#}						
The pressure in kilobars of the Reactive Subsystem (RS). *(1 kbar = 0.1 GPa = 986,92 atm).						
This can be a constant or an expression built using the variables "x i" or "y i", real numbers,						
multiplication(*), division(/),addi	tion(+), subtraction(-) or exponents	(^).				

Temperature (°C)	Numeric/Expression					
{temperature_#}						
The temperature in degrees Celsius of the Reactive Subsystem (RS). $*(1 \circ C = 274.15 \text{ K} = 33.8 \circ \text{F})$						
This can be a constant or an expression built using the variables "x i" or "y i", real numbers,						
multiplication(*), division(/),addi	tion(+),subtraction(-) or exponents	(^).				

# Input File

{pt_def}	String	Options: input
The method of pt definition. *pt c	lefinition from file still to come	

{pt_definitions}	Listed Definition			
Pressure and temperature definition	ons of the form			
pt_definitions<-list("{x_a,y_a}_{	pt_definitions<-list("{x_a,y_a}_{x_b,y_b}]"=c("pressure_#","temperature_#"),			
"{ $x_a,y_a$ }_{ $x_b,y_b$ }"=c("press	ure_#","temperature_#"))			

# Bulk composition

		initiations .
1		
Replace	New	NA2O,MGO,AL2O3,SIO2,K2O,CAO,TIO2,MNO,FEO,NIO,ZRO2,CL2,O2,H2
component	component	0,0,0,0,0,0,0,0,0,0,0,0,5,0,0
02	0	
Major element	s	
NA2O MGO	AL203 SIO2 K	20 CAO TIO2 FEO O H2O
Number of bu	lk definitions	
Number of bu 2 From	lk definitions To	NA20,MGO,AL203,SI02,K20,CA0,TI02,FE0,0,H20,mass
Number of bu 2 From {1;1}	To {1;1}	NA20,MGO,AL203,SI02,K20,CAO,TI02,FEO,O,H2O,mass 1.82,3.28,20.45,56.97,4.09,1.56,1.05,8.5,0.31,1.96,100
Number of bu 2 From {1;1} From	To {1;1} To	NA20,MGO,AL203,SIO2,K20,CA0,TIO2,FE0,O,H20,mass 1.82,3.28,20.45,56,97,4.09,1.56,1.05,8.5,0.31,1.96,100 NA20,MGO,AL203,SIO2,K20,CA0,TIO2,FE0,O,H20,mass

# User interface

Number of Component	Numeric	0<= n_comp_trans	
Transformations			
{n_comp_trans}			
The number of component transformations to apply to the currently available oxide components			
NA2O,MGO,AL2O3,SIO2,K2O,	CAO,TIO2,MNO,FEO,NIO,ZRO2	,CL2,02,H2O,C02	

Replace component	String				
{old_comp_#}					
The current component to replace, options are:					
NA2O,MGO,AL2O3,SIO2,K2O,	CAO,TIO2,MNO,FEO,NIO,ZRO2	,CL2,02,H2O,C02			

New component	String	<6 characters, All capitals
{new_comp_#}		
The name of the new component.	This name must consist of less that	n 6 characters and must be all in
capital letters.		

NA2O,MGO,	Comma-separated numeric	
{comp_#}		
The value of the new component	as a factor of the components :	
NA2O,MGO,AL2O3,SIO2,K2O,	CAO,TIO2,MNO,FEO,NIO,ZRO2,	,CL2,02,H2O,C02. This must be
a string of 15 comma separated nu	umbers of which a total of no-more	-than 11 can be non-zero. For
example, if we wish to use the con	mponent O instead of O2 we would	l use:
0,		
If we wish to use FE2O3 we would	ld use:	
0,0,0,0,0,0,0,0,2,0,0,0,0.5,0,0		

Major elements	Comma-separated-strings				
{major_elements}					
The major element oxides used to define the bulk composition. The available components are :					
NA2O,MGO,AL2O3,SIO2,K2O,	CAO,TIO2,MNO,FEO,NIO,ZRO2	,CL2,02,H2O,C02			

Number of bulk definitions {n bulk def}	Numeric	1<= n_bulk_def
The number of definitions to use	for assigning bulk compositional va	llues.

NA2O,MGO,,mass	Comma-separated-			
	values/expressions			
The wt.% of each elemental ox	ide listed in "Major elements" (a	bove) as well as the relative starting		
mass (in grams) of the Reactive Subsystem (RS).				
Expressions can use real numbers, r operators, x_i, y_i, x_n, y_n and any tuples of the form xs{#;#}				
where xs is any of rs,as,es,fs an	d # uses real numbers, r operator	rs, x_i, y_i, x_n and/or y_n		

Import definitions from file	Boolean	TRUE = Import from file		
{bulk_def_file}		FALSE = definition via input		
Choose whether bulk definitions are read from input or imported from a text file (.txt) located in the				
Inputs folder.				

Bulk file		C	haracter s	string		e.g. bu	ılk.txt		
{bulk_file}									
The name of the in	nput file	containi	ing the bu	ılk compo	sition defi	initions	(the na	me must	end with .tx
The bulk file must	t be a tab	delimit	ed text fi	le (.txt) co	ntaining t	the colui	mns "F	rom", "T	o", your
selection of major	element	s and "N	Aass" Fo	r example				,	<i>,</i> <b>,</b>
serection of major	0101110110	o una m	1455 110	i enampre	•				
📃 bulk.txt - Notepad						—		×	
<u>File Edit Format</u>	<u>/</u> iew <u>H</u> elp								
FROM TO	NA20	MGO	AL203	SI02	CAO	FE0	MASS	~	
1:1 1:2	0.53	25.8	6.93	48.15	7.02	10.93	100		
1;1 1;2 This text file can be seen to be s	0.53 be easily	25.8 exported	6.93 d from ar	48.15 n excel file bulk.xlsx - Excel	7.02 e using Fi	10.93	100 As\Tex	xt (tab del	imited) (*.tz
1;1 1;2 This text file can b File Home Inset Page Layou Calibri Copy - Calibri	0.53	25.8 exported sta Review	6.93 d from ar	48.15 excel file bulkatse Excel at you want to do General	7.02 e using Fi © ™	10.93	100 As\Tex	tt (tab del state -1 p> bratt > Popets > tot	imited) (*.tx
1;1     1;2       This text file can be set file can be set file can be set file can be set file for the set for t	0.53	25.8 exported ata Review	6.93 d from ar View Q Tell me wh Wrap Test Wrap Test Merge & Center	48.15	or.02 e using Fi	10.93	100 As∖Tex	tt (tab del bucker) Const (ta	imited) (*.t;
1;1     1;2       This text file can be to	0.53	25.8 exported sta Review	6.93 d from ar View ♀ Tell me wh ☞ Wrap Test ☞ Merge & Center iment	48.15	e using Fi	10.93	100 As∖Tex	transformed and the second secon	imited) (*.t;
1;1     1;2       This text file can be set file can be set file can be set for a calibri be can be set for a calibri be can be set for a calibri be set for a	0.53	25.8 exported ata Review	6.93 d from ar View Q Tell me wh Wrap Test Wrap Test Merge & Center imment	48.15	7.02 e using Fi	10.93	100 As\Tex	ct (tab dell     ctat (tab	imited) (*.t: <sup>a) spots</sup>
1;1       1;2         This text file can be set file can be set file can be set file can be set file for the set format Painter format Painter for the set format Painter format Painter for the set format Painter format Pai	0.53	25.8 exported ta Review	6.93	48.15	7.02 e using Fi wa wa wa wa wa wa wa wa	10.93	100 As\Tex	constraints and a second	imited) (*.tz
1;1     1;2       This text file can be set file can be set file can be set file to the set file can be set file to the set file t	0.53 De easily t Formulas D 11 A A A FROM D E AL203	25.8 exported ata Review F = = = = = = Altor	6.93 d from ar Wrew Q Tell me wh Wrap Test Merge & Center Merge & Center	48.15 Dulkads - Excel at you want to do General Solution Number	7.02 e using Fi o o o o o o o o o o o o o o o o o o o	10.93	100 As\Tex	constraints and a second	imited) (*.tz
1;1       1;2         This text file can be set file can be set file can be set file can be set file for the set for the set for the set file for the set for the set file for the set for the	0.53	25.8 exported ta Review E = = • • • • Align Slo2 Slo2 CAC 3 48.15 9 48.08	6.93 d from an Wew ♀ Tell me wh Wrape & Center Merge & Center Merge & Center Merge & Center 7.00 10.93 7.76 11.23	48.15	7.02 e using Fi we we we we we we we we we we we we we	10.93	100 As\Tex	Comparison of the second	imited) (*.tz
1;1       1;2         This text file can be set file can be set file can be set file can be set file for the set file for the set fo	0.53	25.8 exported ata Review F = 0 0 0 F = 0 0 Align Align SiO2 CAC 3 48.15 9 48.08 1 48.76	6.93 d from an Wew ♀ Tell me wh ☞ Wrape & Center ment	48.15	7.02 e using Fi we we we we we we we we we we we we we	10.93	100 As\Tex	Comparison of the second	imited) (*.t;

The bulk definitions describe the wt.% of each elemental oxide as well as the relative starting mass (in grams) of the Reactive Subsystem (RS). Expressions can use real numbers, r operators, x\_i, y\_i, x\_n, y\_n and any tuples of the form  $xs{#;#}$  where xs is any of rs,as,es,fs and # uses real numbers, r operators, x\_i, y\_i, x\_n and/or y\_n

Phase Addition         Phase Addition         Perform Phase Addition?         Number of addition definitions         1         From       To         H20,SI02,AL203,CA0,MG0,FE0,K20,NA20,TI02,0,mass	Ph	ase Manipu	lations	
Phase Addition          Perform Phase Addition?         Number of addition definitions         1         From       To         H20,SI02,AL203,CA0,MG0,FE0,K20,NA20,TI02,0,mass	Pha	ase Addition	1	
From To H2O,SIO2,AL2O3,CAO,MGO,FEO,K2O,NA2O,TIO2,O,mass		Phase Addition Perform Phane Number of addition	ase Addition?	
		From	То	H2O,SIO2,AL2O3,CAO,MGO,FEO,K2O,NA2O,TIO2,O,mass
{1;1} {30;1} 0,62.9908959646287,23.2551099914014,4.48742666854471,0,0		{1;1}	{30;1}	0,62.9908959646287,23.2551099914014,4.48742666854471,0,0

## User interface

Perform Phase Addition?	Boolean	TRUE/FALSE			
{ph_add}					
Add phases/components into the Reactive Subsystem (RS) at specified points?					

Number of addition definitions	Numeric	
{n_ph_add_def}		
The number of definitions to use	for assigning phase additions.	

#,#,mass	Comma-separated-values				
The wt.% of each elemental oxide listed in "Major elements" (Bulk composition tab) as well as the					
relative starting mass (in grams	) of the phases/components to ac	ld.			

## Phase Extraction

Phase Extra	ction		
Perform F	Phase Extraction?		
Phases for	extraction		
Melt			
Number of e	extraction definitio	ns	
1			
From	То	Condition	
{1:1}	{25;1}	Melt,>=,7,wt%	
Met			
100%			

#### User interface

Perform Phase Extraction?	Boolean	TRUE/FALSE			
{ph_extr}					
Extract phases from the Reactive Subsystem (RS) when specified criteria are met?					

Phases for extraction	Comma-separated-strings				
{extr_phases}					
Phases to be considered for phase extraction. These can be from the list of solution models chosen					

(Phase Models tab) or any pure phase output by Perple\_X (see <u>Perple\_X Solution Model Glossary</u>) and <u>THERMOCALC's list of mineral abbreviations</u>)

Number of extraction	Numeric				
definitions					
{n_ph_extr_def}					
The number of definitions to use for assigning phase extractions.					

Condition	Logical/expression	Options:			
		TRUE			
		FALSE			
		melt(HP),>=,7,wt%			
A conditional argument of the f	<pre>Form {phase},{condition},{value</pre>	e},{unit}			
For example to extract phases w	stract phases whenever melt exceeds a 7 vol% threshold you would use the following				
condition: melt(HP),>=,7,vol%					

[Phase values]		Numeric/expression			Must not be allowed to be greated						ter		
					than t	he amo	ount	prese	ent				
	 0 1		1 1	1 1.	(( <b>D</b> 1	C		. •		ъ			

Define the proportion of phase to extract for each phase listed in "Phases for extraction". Proportions can be given as:

- 1. A percentage of what is present (e.g. 10%) \*you must include the percentage sign for this
- 2. A set mass (in g) relative to the full system (100g).
- 3. For melt the expression retain(value, unit) allows extraction to occur until a set amount of melt is left behind where value is the amount and unit is either wt% or vol%.

#### Modelling Options

Modelling Data

Modelling Data	
Thermodynamic Data File	
hp04ver.dat	
Solution Models File	
solution_model.dat	
Perple_X Option File	
perplex option.dat	

#### **User interface**

Thermodynamic Data File	String	Default = hp04ver.dat			
{thermodynamic_data_file}					
The thermodynamic data file pr	ata file present in ~Rcrust/bin/data to be used for phase stability calculations.				

Solution Models File	String	Default = solution_model.dat			
{solution_models_file}					
The solution model file present in ~Rcrust/bin/data from which solution models can be chosen.					

Perple_X Option File	Strings	Default = perplex_option.dat	
{perplex_option_file}			
The perplex option file present in ~Rcrust/bin/data which controls extra settings for phase stability			
calculations.			

# Phase Models

Solution mo	dels								
feldspar Bi Mt(W)	o(TCC)	hCrd	Gt(WPH)	Opx(HP)	Cpx(HP)	llm(WPH)	melt(HP)	Mica(CHA)	Sp(HP)
Melt model									
melt(HP)									,

Solution models	Comma-separated-strings		
{use_sol_models}			
The solution models to use in phase stability calculations sourced from the Solution Models File.			
(see <u>Perple_X Solution Model Glossary</u> for details)			

Melt model	String	Default = melt(HP)
{melt.name}		
The solution model to use for n	nelt.	

# Outputs

Phase Aliases	Comma separated strings	e.g. TiBio(HP)=Bt,Gt(WPH)=Gt		
{ phase_aliases }				
A list of aliases to use for renaming phases of the form TiBio(HP)=Bt,Gt(WPH)=Gt,etc.				
To hide a phase from plotting use the alias "hide" e.g. TiBio(HP)=hide.				

Select Output = Data File

Select Output = Grid

Select Output = Phase Abundance Along Path

Select Output = PAM

# File Management

Functions for file management. See Rcrust File management for more details

Projects Directory	String	
{projects_directory}		
Absolute location of the projects	directory within the Rcrust folder.	

Working File	String	{1;1}<=
{working_file}		pt_from_#<={x_n;y_n}
Name of the current file under op	eration. Each file has its own folder	r within the projects directory

# containing results of simulations (#.RData file), "Inputs" and "Outputs".

Save	Function call	
{on_save}		
Saves the current GUI inputs and	workspace to the working_file.	

Load	Function call	
{on_load}		
Loads the previously saved worki	ng file into the GUI inputs and wo	rkspace.

Run	Function call	
{manual_load}		
Saves the current GUI inputs and	workspace to the working_file. Th	en launches the Rcrust
calculation	-	

Clear	Function call	
{on_clear}		
Clears the current GUI inputs and	workspace.	

Close	Function call	
{stopApp}		
Closes the current GUI to allow in	nteraction with the R console. To re-	elaunch the Rcrust GUI type
'runApp()' then press [Enter].		

## Perple\_x options

## Options parsed to wrapper calculation set in init\_meem.r

Number of chemical	Integer	Default = 15
components		
{number_components}		
The number of chemical components to build the major elements from.		

Unit for bulk	Integer	0 = molar %
composition		1 = weight %
definition		Default = 1
The unit proportion to use for bulk composition definition.		

## Advanced user options

# Static variable options accessible through main.r

Calculation mode	Character vector	normal
{calc_mode}		Default = normal
Advanced setting toggling the calculation mode.		

PT definition	Character vector	input
{pt_def}		Default = input
Advanced setting toggling the PT definition mode. Used to allow PT definition from file.		

Reaction buffering	Boolean	T (TRUE)
{reaction_buffering}		F (FALSE)
_		Default = FALSE
Allows reaction buffering (threshold buffering) whereby phase extractions set on conditions are		
postponed by the number of reaction buffer steps to ensure continued exceedance of the threshold.		

# **Commands in the R console**

Running Rcrust

Relaunch GUI	Function call	
{.First()} or {Rcrust()}		
Relaunches the Rcrust GUI from	the R console	

Manually initiate calculation	Function call	
Sends the current working file to	be calculated	

# Outputs

Data file {data_file()}	Function call	
Compiles calculation results into	a table	

Write data file	Function call	
{write_data_file}		
Writes compilation table to file		

Grid data	Function call	
{grid_data()}		
Compiles an X Y grid of the value	es of a given variable	

Write grid file	Function call	
{write_grid_file}		
Writes X Y grid to file		

# **Useful functions in the R Console**

ls() List all objects in the current environment

Q() Quits

[Ctrl]+[w] Toggles buffering of outputs

**Rcrust()** Manually launches the Rcrust GUI

To access the R console out of a browser click anywhere in the R console window and press [esc]. This will close the Rcrust GUI which has current control over the console. To relaunch the Rcrust GUI at any time simply type runApp() and press [enter].

#### Rcrust variables

PT[[bulk]][[step]]\$press\$temp	list
List of pressure and temperature conditions for each step in each bulk	

# crust[[bulk]][[step]][phase,detail]listThe full system (FS). Contains details of the reactive subsystem (RS) at each step along with<br/>cumulative extract (ES) and addition (AS) subsystems. Phases in crust are reported as cumulative<br/>weighted averages.

#### c0[detail]

Bulk composition passed between points

workingfile	Character vector
The current Working File	

work_dir	Character vector
The current Working Directory. This is the location of the folder containing the Wo	rking File

vector

## **Development**

Developers of new features should know a few things on the structure of the code. When developing custom functions please stick to these conventions.

The following files are required; they must all be in the same directory (these are contained within the Rcrust folder which should simply be copied to the desired location):

- 1) From **Perple\_X** suite (in a folder called "data"):
  - a. The various datafiles you wish to use, these include: thermodynamic datafiles and solution model files, typically *hp04ver.dat* and *solution\_model.dat* as well as the Perple\_X option file, *perplex\_option.dat*.
  - b. The rest of perple\_x (vertex, build, werami, etc) are not required.
- 2) From **Rcrust** (directly in the "bin" folder):
  - a. ui.r and server.r, these build the Rcrust Graphical User Interface (GUI)
  - b. *main.r*, this houses the main calls to run Rcrust
  - c. Various init\_xxx files, used to transform user input in data structures that Rcrust can understand.
    - i. *init\_bulk.r* sets the bulk composition(s) of the system
    - ii. *init\_pt.r* sets the PT conditions for each step/bulk combination
    - iii. *init\_ph\_add.r* sets the phases to add
    - iv. *init\_ph\_extr.r* sets the phases to extract
    - v. *init\_mem.r* writes user inputs into a meemum build file
    - vi. *init\_dependene* determines the calculation order of points using the depedences assigned
    - vii. *init\_wrapper* loads the compiled phase stability calculator from Perple\_X

d. *parse\_meem*, a temporary Perple\_X build file created to pass data into the wrapper e. *run.Rcrust.r*, the Rcrust calculation loop to be called for each point

Technically, each function works c0 which tracks the bulk compositional changes invoked by phase manipulations. main.r loops through each point, calculating and modifying the phases according to the chosen definitions and eventually stores the final product in a list called crust, whose structure is crust[[y\_i]][[x\_i]]. So, for instance the SiO2 content in the melt of point y\_i=4 and x\_i=2 is

crust[[4]][[2]]["melt(HP)","SIO2"] (assuming you use melt(HP) of course).

f. Various *xxx.dll* files which contain compiled libraries needed to perform calculations within R

# Troubleshooting

A list of known errors that are unavoidable or are still to be fixed.

#### Bulk\_ss system properties

Warning: some bulk system properties are reported as molar properties but perplex considers the bulk system to be one mol thus all molar properties need to be adjusted accordingly

#### Molar phase proportions

Only weight definitions of bulk and phases is currently possible, read.meemum cannot read molar phase proportions. If molar proportions for bulk are entered then bulk is molar but individual phases are weights thus phase extractions crash.

#### Buffered Output

The R console by default returns a buffered output which forces the console to only refresh when flush.console() is called. To disable the buffering and view run data live deselect from R toolbar Misc/Buffered Output.

# REFERENCES

Mayne, M. J., Moyen, J. F., Stevens, G., & Kaislaniemi, L. (2016). Rerust: a tool for calculating pathdependent open system processes and application to melt loss. *Journal of Metamorphic Geology*, **34**(7), 663-682