



Geochemistry, Geophysics, Geosystems

Supporting Information for

REEBOX PRO: A Forward Model Simulating Melting of Thermally and Lithologically Variable Upwelling Mantle

Eric L. Brown¹ and Charles E. Lesher^{1,2}

¹ Department of Geoscience, Aarhus University, Høegh-Guldbergs Gade 2, 8000 Aarhus C, Denmark

² Department of Earth and Planetary Sciences, University of California, Davis, 1 Shields Avenue, Davis, CA 95616 USA

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Introduction

This supporting information is the user guide for REEBOX PRO.

- **Text S1** provides download and installation information
- **Text S2** describes the REEBOX PRO user interface and functionality (Figures S1-S11)
- **Text S3** describes the formats for user-specified input files (Figures S12-S17)
- **Text S4** presents the structure of the model output files (Figures S18-S21)
- **Text S5** provides two worked examples to help familiarize the user with the program
- **Input File S1. TE_iso_input.txt** is an example file for inputting user-specified trace element + isotope compositions into REEBOX PRO
- **Input File S2. per_harz_kd_input.txt** is an example file for inputting user-specified mineral-melt partition coefficients for the peridotite/harzburgite lithologies in REEBOX PRO
- **Input File S3. pyx_kd_input.txt** is an example file for inputting user-specified mineral-melt partition coefficients for the pyroxenite lithologies in REEBOX PRO

Text S1. Download and Installation

REEBOX PRO is provided as a standalone executable program compiled in MATLAB. **You do not need MATLAB, nor knowledge about the MATLAB programming language to run REEBOX PRO.** Instead, the program is distributed with the appropriate MATLAB runtime libraries. The **REEBOX PRO** installation program can be downloaded at <http://volcano.au.dk/reebox-pro/>.

The **REEBOX PRO** installation program is packaged with the necessary runtime libraries. Because the Mac and PC compilers differ, you will need to download a platform-specific installation program (**REEBOX_PRO_v1_Installer_Mac.app** for Mac; **REEBOX_PRO_v1_Installer_PC.exe** for PC). Even if you have MATLAB installed on your computer, you still need to use the installation program because the program was compiled using MATLAB 2016a- the program will only run if the 2016a runtime libraries are installed on the destination computer. The installation program will determine whether these have already been installed and will only install the runtime library if necessary. This means that installation of the (2016a) runtime libraries is a one-time occurrence.

Upon opening the installation program, MATLAB will guide you through a series of installation screens. To ensure that **REEBOX PRO** runs properly on your computer, we recommend you use the default settings suggested by the installation program. The installation program will determine whether or not the runtime libraries need to be installed, install them if necessary, and will then install **REEBOX PRO** in either the *Applications* folder (Mac) or *Program Files* folder (PC) (assuming you followed the default installation options). Once installed, you can find **REEBOX PRO** in ***/Applications/REEBOX PRO/application/REEBOX_PRO.app*** on Mac, or ***/Program Files/REEBOX PRO/application/REEBOX_PRO.exe*** on PC. Double-click on the application to run the program. At present, **REEBOX PRO** runs successfully on Mac OSX Yosemite and El Capitan, and Windows 7 and 10. If you encounter any installation difficulties, please contact Eric Brown (ericlb@geo.au.dk).

Text S2. Using REEBOX PRO

GENERAL TIP: press enter or tab after entering a number in a text box, otherwise the program may not register the change.

S2.1. About REEBOX PRO Window

Upon opening, **REEBOX PRO** displays information about previous versions of the REEBOX program and how to cite use of **REEBOX PRO** (Figure S1). To open the main program window, click **OK**. (Note: all screenshots are from the Mac version of **REEBOX PRO**.)

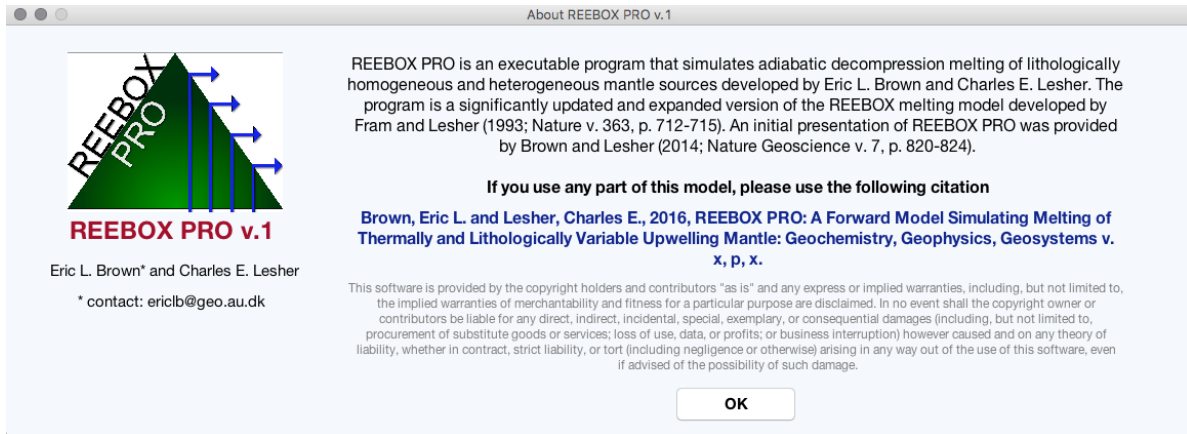


Figure S1. *About REEBOX PRO* window, highlighting previous work in developing **REEBOX PRO** and the appropriate citation for use of the program. Click **OK** to enter the main program window.

S2.2. Main Program Window

Most interactions with **REEBOX PRO** will be via the main program window (Figure S2). Depending upon the size of your display, the sides of this window can be dragged to resize the window. The main program window is divided into five main areas: *Source Lithology Inputs*, *Other Inputs*, *Messages*, *Model Execution*, and *Output Results*, which allow you to manage primary model inputs and outputs, receive feedback about variable changes and/or program errors, and run model calculations. Information about the components displayed in the main program window can be found by hovering the mouse cursor over any of the buttons, text boxes, dropdown menus, and checkboxes (this information can be toggled on and off under the *File* menu → *Turn Hover Text On/Off*). Details of the five main sections are provided below.

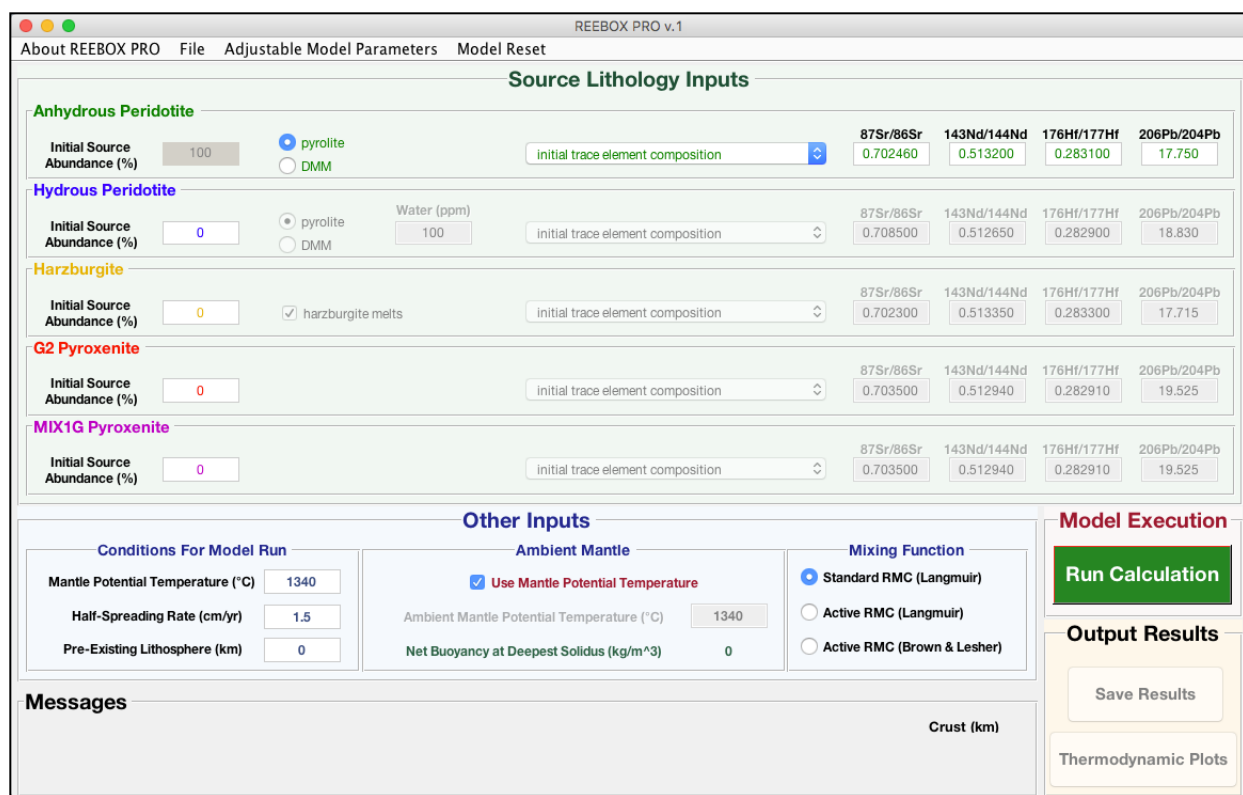


Figure S2. Main program window divided into sections: *Source Lithology Inputs*, *Other Inputs*, *Messages*, *Model Execution*, and *Output Results*.

S2.2.1. Source Lithology Inputs

REEBOX PRO is a tool that can simulate the adiabatic decompression melting behavior of 5 different rock types (anhydrous peridotite, hydrous peridotite, harzburgite, G2 pyroxenite, and MIX1G pyroxenite). These lithologies can be treated either individually (i.e. as a homogeneous source consisting of 100% of any selected lithology), or can be treated together (i.e. as a heterogeneous source consisting of up to all 5 lithologies, where the sum of the selected lithologies abundances is 100%).

The *Source Lithology Inputs* section of the main window is subdivided into five subpanels, where the user can specify the initial source abundance and initial composition of the lithologies incorporated in REEBOX PRO (anhydrous peridotite, hydrous peridotite, harzburgite, G2 pyroxenite, and MIX1G pyroxenite). Common to each of the five panels are the initial source abundance (Φ_i^0 ; input as %), the initial trace element composition (input in ppm), and the initial $^{87}\text{Sr}/^{86}\text{Sr}$, $^{143}\text{Nd}/^{144}\text{Nd}$, $^{176}\text{Hf}/^{177}\text{Hf}$, and $^{206}\text{Pb}/^{204}\text{Pb}$ compositions of the lithology. The program initially assumes the source consists of 100% anhydrous peridotite (Figure S2). Because none of the other lithologies have been

identified as being present in the source (i.e. their initial source abundances are 0%), the compositional inputs for those lithologies are greyed out and cannot be modified. Once a non-zero initial source abundance has been specified for a lithology, the compositional inputs become active and can be modified. If the sum of the initial source abundances of hydrous peridotite, harzburgite, G2 pyroxenite and MIX1G pyroxenite specified by the user do not sum to 100%, REEBOX PRO rounds out the source by adding sufficient anhydrous peridotite to make the source lithologies sum to 100%. If the sum of the initial source abundances is >100%, the program will display an error message.

Options for the initial trace element composition are listed in a drop-down menu, which has been pre-populated with some possible initial trace element compositions that might be relevant for the lithology. For anhydrous/hydrous peridotite and harzburgite, these include an estimate for primitive mantle, two estimates for depleted MORB mantle, and an estimate for depleted-depleted MORB mantle. For G2 pyroxenite and MIX1G pyroxenite, these include two estimates each for NMORB and EMORB. Also included in the initial trace element composition drop-down menu is an option for the user to input their own initial trace element composition. To use this option, the user should prepare a text, tab-delimited file containing the initial trace element (\pm initial isotopic) compositions. This file may contain header row(s) and/or header column(s) (although they are not necessary; see **Text S3.1**).

The panels for anhydrous peridotite, hydrous peridotite, and harzburgite also provide additional inputs beyond those described above. For anhydrous and hydrous peridotite, the user can specify whether the peridotite is more fertile (pyrolite button) or depleted (DMM button) in composition. For hydrous peridotite, the user can also input the initial water content of the peridotite (in ppm). Finally, for harzburgite, the user can specify whether or not the harzburgite melts. If the *Harzburgite melts* checkbox is checked, the program will simulate harzburgite melting, whereas if the checkbox is unchecked, the harzburgite will not be melted (although the presence of harzburgite in the source will influence the net source buoyancy), and the initial trace element and isotopic composition inputs will become inactive (greyed out).

S2.2.2. Other Model Inputs

In addition to the initial abundance(s) and composition(s) of the lithologies comprising the model mantle source, **REEBOX PRO** also requires the user to specify additional model parameters, including the thermal state (mantle potential temperature), half-spreading rate, thickness of any pre-existing continental lithosphere, the thermal conditions of the ambient mantle, and the manner in which pooled melt compositions are calculated. These inputs are subdivided between three

subpanels (*Conditions For Model Run*, *Ambient Mantle*, and *Mixing Function*) under the *Other Inputs* panel in the lower half of the main program window (Figure S2).

In the *Conditions For Model Run* subpanel, the user specifies the potential temperature of the mantle adiabat being modeled (in °C), the plate half-spreading rate (in cm/yr), and the thickness of any pre-existing continental lithosphere (in km). In the *Ambient Mantle* subpanel, the user can explicitly specify the temperature of the ambient mantle. *This is only important when applying the Brown and Lesher-type residual mantle column (RMC) mixing function*, which relies on a nonzero net source buoyancy. By default, the program assumes that the ambient mantle temperature is the same as the potential temperature specified by the user, as denoted by the checked box *Use Mantle Potential Temperature*. If this box is checked, the program will always use the mantle potential temperature, and the value in the box for *Ambient Mantle Potential Temperature* (°C) cannot be changed. To specify a different ambient mantle potential temperature, uncheck the box for *Use Mantle Potential Temperature*, and enter a new value in the now-available input box for *Ambient Mantle Potential Temperature* (°C). Independent of the choice of ambient mantle potential temperature used, the program automatically calculates the net buoyancy of the model source at the deepest solidus based on the specified initial lithologic abundances, mantle potential temperature, and ambient mantle potential temperature. This is shown in green as *Net Source Buoyancy at Deepest Solidus* (kg/m^3). From the program's viewpoint, the net source buoyancy is only significant for the Brown and Lesher RMC calculation, which requires a nonzero (i.e. positive) net source buoyancy.

The user's choice for mixing function is given in the *Mixing Function* subpanel. Here, three options are provided: *Standard (Langmuir) RMC*, *Active (Langmuir) RMC*, and *Active (Brown & Lesher) RMC*. The *Standard (Langmuir) RMC* option pools all melts assuming passive upwelling through a triangular melting zone, using the residual mantle column method presented by *Langmuir et al.* [1992]. The *Active (Langmuir) RMC* option pools all melts assuming end-member active upwelling induced by buoyancy effects during melting and/or melt retention. This calculation assumes all melting columns decompress to the base of the crust/lithosphere, and is based on the residual mantle column method presented by *Langmuir et al.* [1992]. The *Active (Brown & Lesher) RMC* option pools all melts assuming active flow through the melting zone due to intrinsic buoyancy of the source prior to entering the melting zone (e.g. enhanced buoyancy due to a thermal anomaly/plume). This calculation combines the residual mantle column method of *Langmuir et al.* [1992] and the residual mantle cylinder method of *Ito and Mahoney* [2005], as presented by *Brown and Lesher* [2014].

S2.2.3. Messages

In the *Messages* panel, error messages are displayed in red, and program update messages are displayed in blue. Error messages most commonly result from improper inputs into the text boxes (i.e. non-numeric values or leaving the text box empty), sources consisting of >100% of specified lithologies, or attempting to use the *Active (Brown & Leshner) RMC* mixing function when the net source buoyancy is not positive. Program errors such as these also result in a pop-up window indicating the error (Figure S3).

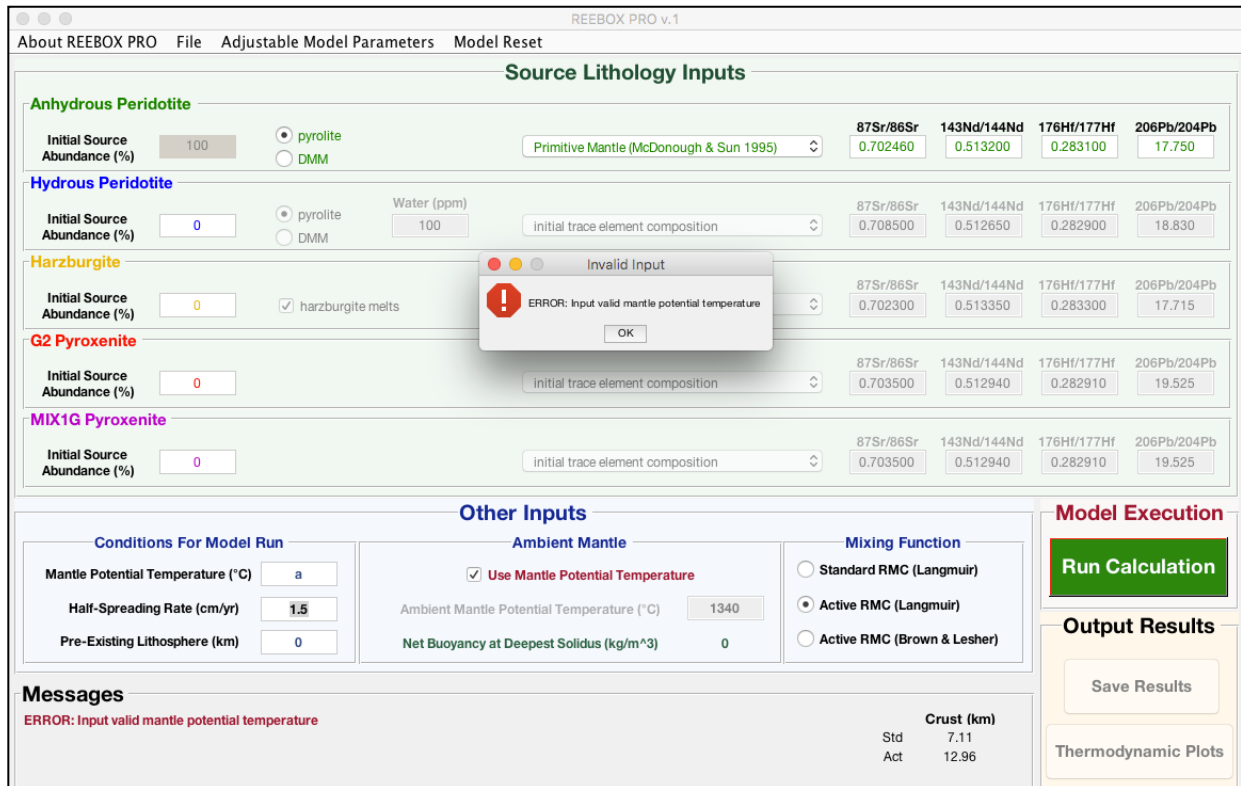


Figure S3. Error message example. Inputting an invalid number (see Mantle Potential Temperature input) results in an error message pop-up and an error message shown in red in *Messages* panel.

Program update messages display the most recent user action that resulted in a change to a model input (Figure S4), the start of a model run, or at the return of a successful model run. Furthermore, after the program completes a successful run, the right-hand portion of the *Messages* panel will display the igneous crustal thickness calculated using the specified mixing function. If either of the active mixing functions are selected, the crustal thickness calculated using the *Standard (Langmuir) RMC* mixing function is also shown (for comparative purposes; see Figure S4).

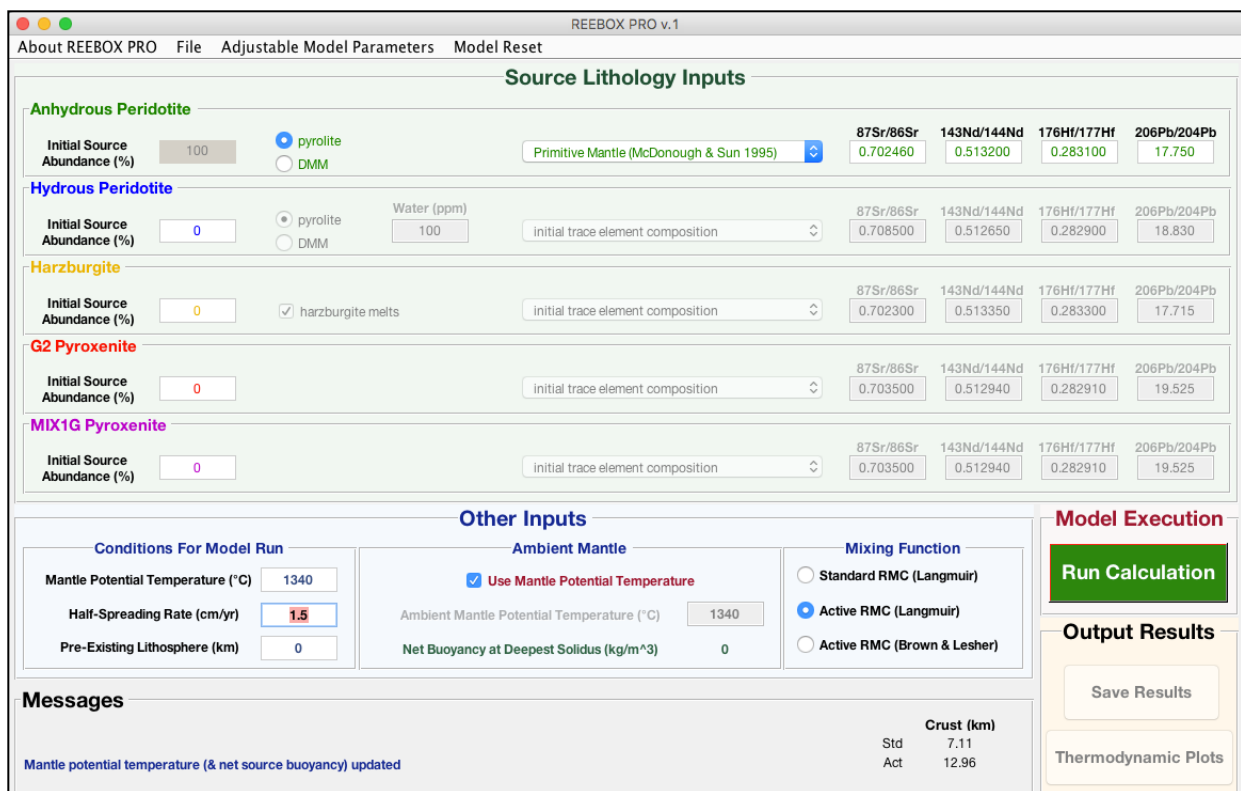


Figure S4. Program update message shown in blue at bottom of the **Messages** panel. In this case, the mantle potential temperature has been adjusted.

S2.2.4. Model Execution

Once all model inputs have been specified, the user can run REEBOX PRO by clicking the green *Run Calculation* button in the *Model Execution* panel (Figure S2). Once clicked, the program checks for any input errors, and if none exist, executes the melting calculation (*Program is running. Please be patient...* will appear in the *Messages* panel). While the calculations are being performed, the *Run Calculation* button will become unavailable (greyed out) to prevent inadvertent rerunning of the model. Once the calculation finishes (or results in an error), the *Run Calculation* button becomes available again.

S2.2.5. Output Results

Upon opening the program, or after changing model inputs or parameters, the *Save Model Results* and *Make Thermodynamic Plots* buttons are inactive (Figure S4). However, these buttons become active once a model runs successfully. The program provides two different forms of model output. Clicking the *Save Results* button in the *Output Results* panel generating an output folder,

which includes tab-delimited text files containing all model inputs and results (instantaneous melt compositions, column-accumulated melt compositions, and pooled melt compositions derived from each specified lithology, as well as the bulk crustal composition calculated using the specified mixing function). After clicking the *Save Results* button, the user is prompted to navigate to the directory/folder where they would like the output folder to be saved. Once this is selected, the program outputs the results into a folder named **REEBOX_PRO_OUTPUTS**, appended with the date and time in *_yyyy_mm_dd_hh_mm_ss* format (e.g. **_2016_5_3_12_50_49**). In this way, **REEBOX PRO** should never overwrite previous model outputs.

The output folder contains a folder named for the specified mixing function (e.g. *Standard_RMC_Langmuir* in the example shown in Figure S5). This folder contains the text file for the bulk crustal composition calculated using the specified mixing function, along with folders for the instantaneous melt compositions, column-accumulated melt compositions, and pooled melt compositions for all specified lithologies (Figure S5). All output files can be opened and manipulated in Microsoft Excel, and ***all files have the same structure***. See **Text S4** for more details about the output file structure.

Clicking on the *Make Thermodynamic Plots* button will generate a pop-up figure window that plots (a) the adiabat (black dashed curve), melting path (thick black curve) and the solidi of all specified source lithologies (colored curves) in P-T space; (b) the polybaric productivity of each lithology as a function of pressure; and (c) the total extent of melting of each lithology as a function of pressure (Figure S6). This figure can be resized by dragging the edges of the figure window, and can be saved by clicking the disk icon, or using the *Save* option in the *File* menu. Alternatively, the figure may be printed by clicking the printer icon (or using the *Print* option in the *File* menu).

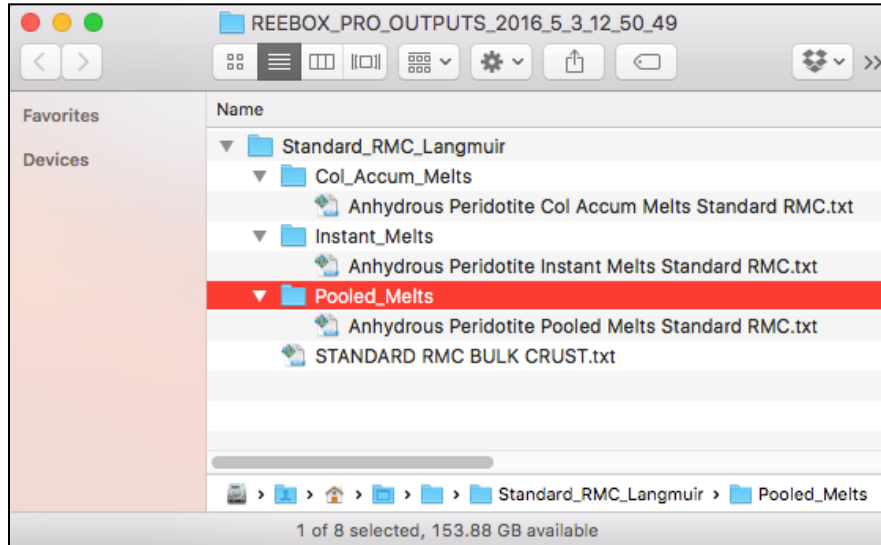


Figure S5. Output folder containing bulk crustal composition output file (*STANDARD RMC BULK CRUST.txt*), along with folders for instantaneous melt (*Instant_Melts*), column-accumulated melts (*Col_Accum_Melts*), and pooled melts (*Pooled_Melts*), which each contain a text file for each specified source lithology (in this case, anhydrous peridotite was the only source lithology specified). In this example, the *Standard (Langmuir) RMC* mixing function was used (see top folder and file names).

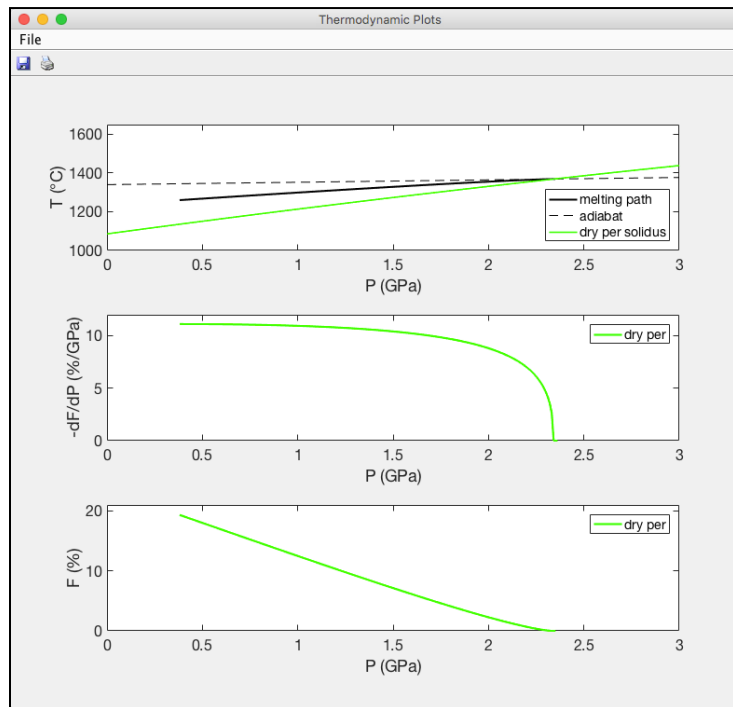


Figure S6. Example of the *Thermodynamic Plots* figure output.

S2.3. Menu Options in the Main Program Window

Four menu options exist in the main program window: *About REEBOX PRO*, *File*, *Adjustable Model Parameters*, and *Model Reset*. For efficiency, most menu options have a hotkey associated with them, which is listed next to the menu item (listed in parenthesis below).

S2.3.1. About REEBOX PRO Menu

The *About REEBOX PRO* menu option brings up the *About REEBOX PRO* window described in Text S2.1 (Figure S1).

S2.3.2. File Menu

The *File* menu provides two options. The first, *Turn Hover Text On/Off*, allows the user to toggle on and off the information displayed when the cursor hovers over any of the buttons, text boxes, dropdown menus, and checkboxes. The second option, *Close Program (Q)*, exits the program.

S2.3.3. Adjustable Model Parameters Menu

The *Adjustable Model Parameters* menu allows users to change the default values used for the key parameters used in the model calculations. This menu has four options (*Thermodynamic Parameters (T)*, *Viscosity Parameters (Brown & Lesher RMC) (F)*, *Lithosphere Parameters (L)*, and a *Partition Coefficients* submenu). The options/menus within the *Adjustable Model Parameters* menu are described in more detail below.

Thermodynamic Parameters (T)

The *Thermodynamic Parameters (T)* menu option under the *Adjustable Model Parameters* menu brings up the *Thermodynamic Parameters* window containing the thermodynamic inputs used in the model melting calculations (Figure S7). The thermodynamic variables are divided between two panels: *Entropy Change Upon Melting*, and *Other Variables*. The *Entropy Change Upon Melting* panel allows the user to specify the entropy change upon melting (ΔS_{fusion}) for each source lithology. The *Other Variables* panel contains entries for isobaric specific heat capacity (C_p^S), coefficient of thermal expansion (α^S), and the density of basaltic crust (ρ_{crust}). Clicking the *Use Defaults* button restores the thermodynamic parameters to their model default values. Clicking the *OK* button exits the window and returns the user to the main program window.

Entropy Change Upon Melting	
Anhydrous Peridotite ($\Delta S_{fusion_{dry_per}}$) [J/(kg K)]	300
Hydrous Peridotite ($\Delta S_{fusion_{wet_per}}$) [J/(kg K)]	300
Harzburgite ($\Delta S_{fusion_{harz}}$) [J/(kg K)]	300
G2 Pyroxenite ($\Delta S_{fusion_{G2_pyx}}$) [J/(kg K)]	240
MIX1G Pyroxenite ($\Delta S_{fusion_{MIX1G_pyx}}$) [J/(kg K)]	240

Other Variables	
Isobaric Specific Heat capacity (C_P^S) [J/(kg K)]	1200
Coefficient of Thermal Expansion (α^S) [1/K]	3.00e-05
Density of Basaltic Crust (ρ_{crust}) [kg/m ³]	2800

Buttons: Use Defaults, OK

Figure S7. *Thermodynamic Parameters* window.

Viscosity Parameters (Brown & Leshar RMC) (F)

The *Viscosity Parameters (Brown & Leshar RMC) (F)* menu option under the *Adjustable Model Parameters* menu brings up the *Viscosity Parameters* window containing the viscosity inputs used in the **Active (Brown & Leshar) RMC** mantle flow calculations (Figure S8). These inputs are the reference viscosity (η_0), activation energy (E_{act}), activation volume (V_{act}), and reference pressure (P_{ref}). Clicking the *Use Defaults* button restores the viscosity parameters to their model default values. Clicking the *OK* button exits the window and returns the user to the main program window.

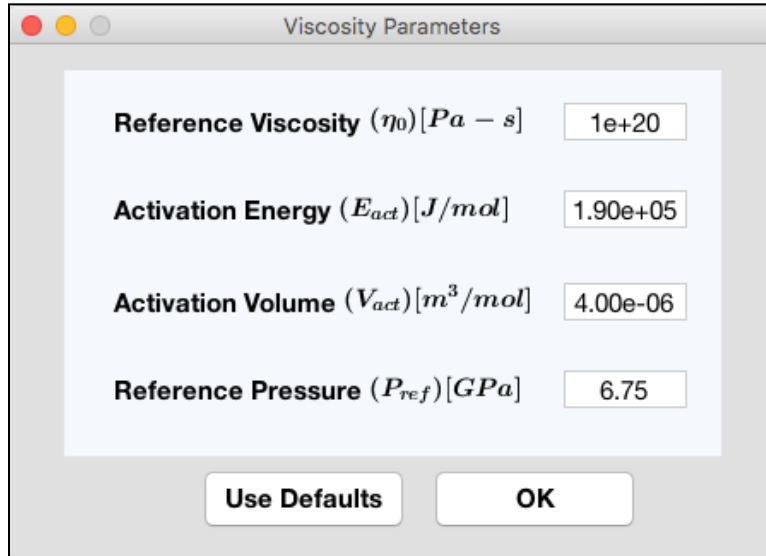


Figure S8. Viscosity Parameters window.

Brown and Lesher RMC Buoyancy Threshold (B)

The *Brown and Lesher RMC Buoyancy Threshold (B)* menu option under the *Adjustable Model Parameters* menu opens the *Minimum Net Buoyancy (Brown & Lesher RMC)* window containing the minimum net source buoyancy required for application of the Active (Brown & Lesher) RMC mixing function, when this mixing function is selected (Figure S9). If the Active (Brown & Lesher) RMC mixing function is selected (i.e. the net source buoyancy is > 0 kg/m³) and the calculated net source buoyancy is below this minimum threshold, the mixing calculation will be made using the Standard (Langmuir) RMC.

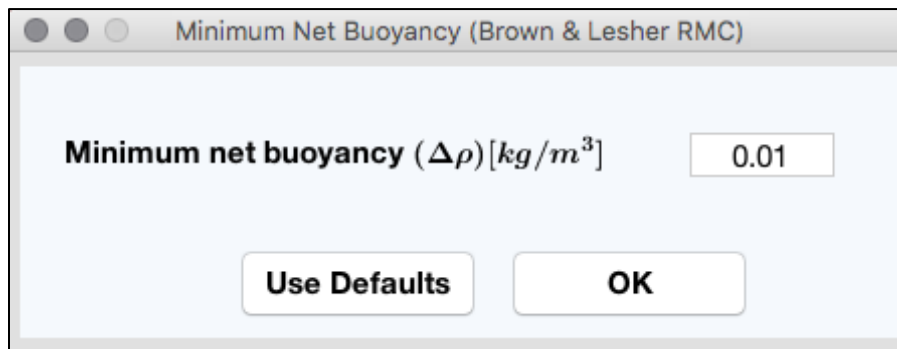


Figure S9. Minimum Net Buoyancy (Brown & Lesher RMC) window.

Lithosphere Parameters (L)

The *Lithosphere Parameters (L)* menu option under the *Adjustable Model Parameters* menu opens the *Lithosphere Parameters* window containing the variables used to calculate the density of any specified pre-existing lithosphere (Figure S10). These inputs include the density of continental crust (ρ_{CC}), the density of lithospheric mantle (ρ_{LM}), and the fraction of continental crust comprising the lithosphere (f_{CC}). The value input for the fraction of continental crust should be between 0 and 1. Clicking the *Use Defaults* button restores the viscosity parameters to their model default values. Clicking the *OK* button exits the window and returns the user to the main program window.

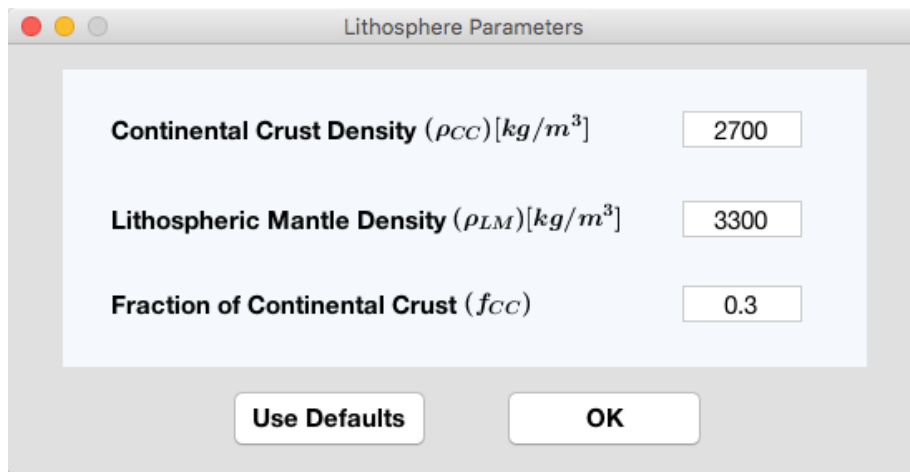


Figure S10. *Lithosphere Parameters* window.

Partition Coefficients Submenu

The *Partition Coefficients* menu option reveals a submenu consisting of three options: *Dry/Wet Peridotite & Harzburgite*, *G2 & MIX1G Pyroxenite*, and *Check Current Partition Coefficients (K)*. These submenus allow the user to specify the partition coefficients used in the model calculations, as well as verify the partition coefficient values currently in use. The key assumption is that the same partition coefficients apply for the anhydrous peridotite, hydrous peridotite, and harzburgite sources. Similarly, the G2 pyroxenite and MIX1G pyroxenite sources use identical partition coefficients (although these are likely different than those used for the peridotite/harzburgite lithologies). The options provided by these submenus are presented below.

Dry/Wet Peridotite & Harzburgite Submenu

The *Dry/Wet Peridotite & Harzburgite* submenu provides three options: *Use T-Dependent Partition Coefficients (Default) (1)*, *Use Built-In Constant Partition Coefficients (2)*, and *Load User-Defined Constant Partition Coefficients (3)*. Choosing the first option, *Use T-Dependent Partition Coefficients (Default) (1)*, results in the model using temperature-dependent partition coefficients for the peridotite/harzburgite lithologies. The second option, *Use Built-In Constant Partition Coefficients (2)*, results in the model employing that constant peridotite/harzburgite partition coefficients built into the program. The third option, *Load User-Defined Constant Partition Coefficients (3)*, allows the user to navigate to a text file containing their own constant partition coefficients, and load these partition coefficients for use in the model. This text file may or may not include a header row or column. An example partition coefficient file is shown in **Text S3.2**.

G2 & MIX1G Pyroxenite Submenu

The *G2 & MIX1G* submenu provides two options: *Use Built-In Constant Partition Coefficients (Default) (4)*, and *Load User-Defined Constant Partition Coefficients (5)*. As with the peridotite/harzburgite partition coefficients described above, choosing the first option, *Use Built-In Constant Partition Coefficients (Default) (4)*, results in the model employing that constant G2/MIX1G partition coefficients built into the program. The second option, *Load User-Defined Constant Partition Coefficients (5)*, allows the user to navigate to a text file containing their own constant partition coefficients, and load these partition coefficients for use in the model. This text file may or may not include a header row or column. An example partition coefficient file is shown in **Text S3.3**.

Check Current Partition Coefficients (K) Option

The *Check Current Partition Coefficients (K)* option produces the *Current Partition Coefficients* window that shows the partition coefficients currently in use by the model (Figure S11). In this window, only constant partition coefficients are displayed (the default, temperature-dependent partition coefficients for peridotite/harzburgite will not be displayed if they are currently in use by the program). Clicking the *OK* button closes this window and returns to the main program window. If the user chooses to load their own partition coefficients, it is good practice to verify that the model has successfully incorporated them using the *Check Current Partition Coefficients (K)* menu option.

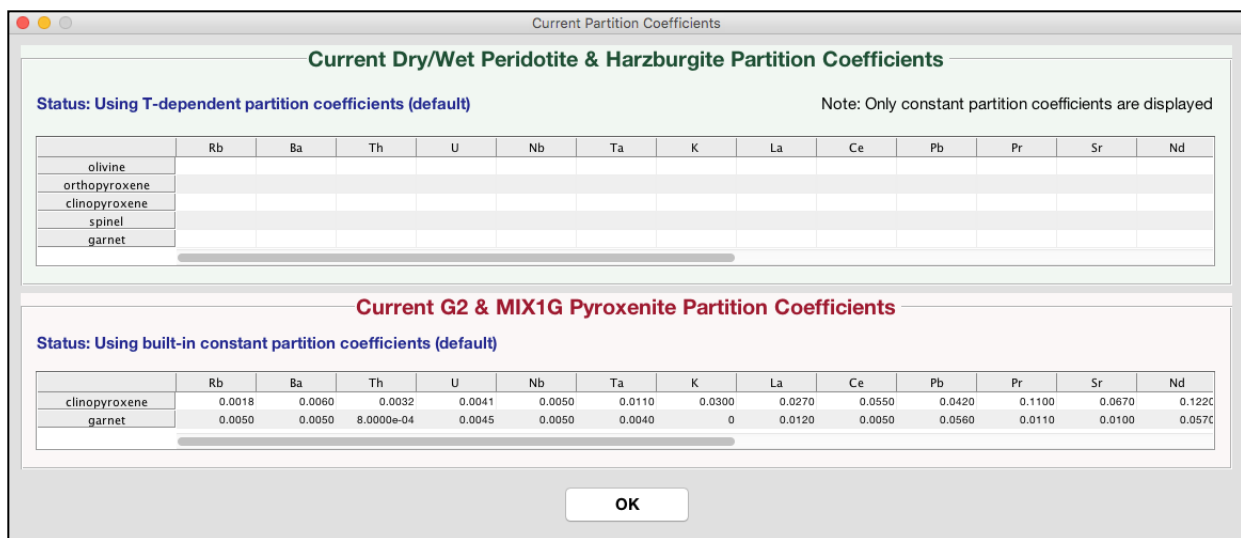


Figure S11. *Current Partition Coefficients* window. Because only constant partition coefficients are displayed, this example (which uses the default temperature-dependent partition coefficients for peridotite/harzburgite) shows no partition coefficients for the peridotite/harzburgite sources.

S2.3.4. Model Reset Menu

The *Model Reset* menu has a single option: *Reset All Model Parameters To Defaults (R)*. This option resets the values of all parameters used in the model to their default values. This option should be used if the user encounters repeated errors (which can arise from improper user-specified parameter values), or would like a fresh start.

Text S3. User-Specified Input File Format and Structures

As noted in Text S2.2.1 and S2.3.3, REEBOX PRO can load user-specified data for the initial trace element/isotope compositions and mineral-melt partition coefficients for peridotite/harzburgite and G2/MIX1G pyroxenite. **In all cases, the input files should be saved as tab-delimited text files.** The appropriate file structures for each of these types of input files are described below.

S3.1. Initial Trace Element ± Isotope Input File

In the *Source Lithology Inputs* panel of the main program window (Figure S2), the user specifies the initial trace element composition of each lithology (with nonzero abundances) using the drop-down menu. When the *user-specified* option is selected, the user is prompted to navigate and open a tab-delimited text file containing the initial trace element composition (± the isotopic compositions) for the lithology (***all trace element compositions should be input as parts per million***

concentrations). As shown in Figure S12, the file may contain a header row (e.g. element/isotope header) and a non-numeric first column (e.g. source name), as well as the initial isotopic compositions. Alternatively, as shown in Figure S13, the file may contain only numeric values (i.e. no header row or non-numeric first column), and only the initial trace element compositions (i.e. no isotopic compositions). Nevertheless, independent of whether the file contains a header or not, the trace elements should **always** be listed in the order Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Ti, Gd, Dy, Y, Er, Yb, and Lu. If isotopes are included in the input file (Figure S12), they should **always** be listed in the order $^{87}\text{Sr}/^{86}\text{Sr}$, $^{143}\text{Nd}/^{144}\text{Nd}$, $^{176}\text{Hf}/^{177}\text{Hf}$, and $^{206}\text{Pb}/^{204}\text{Pb}$. An example trace element and isotope input file (entitled *Input File S1.TE_iso_input.txt*) is included in the *Supporting Information*.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1		Rb	Ba	Th	U	Nb	Ta	K	La	Ce	Pb	Pr	Sr	Nd	Sm	Zr	Hf	Eu	Ti	Gd	Dy	Y	Er	Yb	Lu	87Sr/86Sr	143Nd/144Nd	176Hf/177Hf	206Pb/204Pb
2	example source	0.088	1.2	0.0137	0.0047	0.2104	0.0138	60	0.234	0.772	0.0232	0.131	9.8	0.713	0.27	7.95	0.199	0.107	798	0.395	0.531	4.07	0.371	0.401	0.063	0.704355	0.512155	0.212155	21.345

Figure S12. Example tab-delimited user-specified initial trace element (and isotopic) composition input file containing a header row and non-numeric first column. This file structure is readily input into **REEBOX PRO**.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
1	0.088	1.2	0.0137	0.0047	0.2104	0.0138	60	0.234	0.772	0.0232	0.131	9.8	0.713	0.27	7.95	0.199	0.107	798	0.395	0.531	4.07	0.371	0.401	0.063

Figure S13. Example tab-delimited user-specified initial trace element composition input file containing only the initial trace element compositions. This file structure is readily input into **REEBOX PRO**.

S3.2. Peridotite/Harzburgite Constant Partition Coefficient Input File

In the *Partition Coefficients* submenu of the *Adjustable Model Parameters* menu, the user can choose one of three possibilities for the mineral-melt partition coefficients for the peridotite and harzburgite lithologies. If the *Load User-Defined Constant Partition Coefficients (3)* option is selected under the *Dry/Wet Peridotite & Harzburgite* submenu, the user will be prompted to navigate to and open a tab-delimited text file containing the mineral-melt partition coefficients for the elements Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Ti, Gd, Dy, Y, Er, Yb, and Lu (listed in this order) in each of the minerals olivine, orthopyroxene, clinopyroxene, spinel, and garnet (listed in this order). As shown in Figure S14, this file should consist of 5 rows and 24 columns of numeric data (the rows correspond to the mineral phases; the columns correspond to the elements). As with the initial trace element \pm isotope input file, this partition coefficient file may contain a header row (element header) and/or a non-numeric first column (mineral phase names) (Figure S14). Alternatively, no headers are required, so long as the partition coefficient data are listed in the correct orders given above (with respect to the elements and mineral phases) (Figure S15). An example peridotite/harzburgite constant partition coefficient input file (entitled *Input File S2.per_harz_kd_input.txt*) is included in the *Supporting Information*.

S3.3. G2 & MIX1G Constant Partition Coefficient Input File

In the *Partition Coefficients* submenu of the *Adjustable Model Parameters* menu, the user can choose one of two possibilities for the mineral-melt partition coefficients for the G2 and MIX1G pyroxenite lithologies. If the *Load User-Defined Constant Partition Coefficients (5)* option is selected under the *G2 & MIX1G Pyroxenite* submenu, the user will be prompted to navigate to and open a tab-delimited text file containing the mineral-melt partition coefficients for the elements Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Ti, Gd, Dy, Y, Er, Yb, and Lu (listed in this order) in each of the minerals clinopyroxene and garnet (listed in this order). As shown in Figure S16, this file should consist of 2 rows and 24 columns of numeric data (the rows correspond to the mineral phases; the columns correspond to the elements). As with the initial trace element \pm isotope input file, this partition coefficient file may contain a header row (element header) and/or a non-numeric first column (mineral phase names) (Figure S16). Alternatively, no headers are required, so long as the partition coefficient data are listed in the correct orders given above (with respect to the elements and mineral phases) (Figure S17). An example pyroxenite constant partition coefficient input file (entitled *Input File S3.pyx_kd_input.txt*) is included in the *Supporting Information*.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1		Rb	Ba	Th	U	Nb	Ta	K	La	Ce	Pb	Pr	Sr	Nd	Sm	Zr	Hf	Eu	Ti	Gd	Dy	Y	Er	Yb	Lu
2	olivine	0.00018	0.0003	0.00001	0.0004	0.005	0.0005	0.00002	0.0004	0.0005	0.00001	0.001	0.00019	0.001	0.001	0.01	0.005	0.002	0.02	0.002	0.002	0.005	0.002	0.0015	0.0015
3	orthopyroxene	0.006	0.0006	0.001	0	0.0031	0.004	0.0001	0.002	0.003	0.0013	0.0048	0.007	0.0068	0.01	0.01	0.01	0.013	0.024	0.016	0.022	0.028	0.03	0.049	0.06
4	clinopyroxene	0.0007	0.0007	0.00068	0.0008	0.0077	0.01	0.001	0.0536	0.0858	0.01	0.1	0.13	0.19	0.29	0.12	0.26	0.47	0.38	0.48	0.44	0.4	0.39	0.43	0.43
5	spinel	0	0	0.0024	0.012	0.086	0.08	0	0.0012	0.0019	0	0.0023	0.003	0.01	0.007	0.56	0.65	0.01	0.048	0.016	0.01	0.05	0.01	0.01	0.28
6	garnet	0.007	0.0007	0.0007	0.005	0.02	0.015	0.013	0.01	0.021	0.0005	0.045	0.006	0.087	0.217	0.32	0.32	0.4	0.2	0.498	1.06	2.11	3	4.03	5.5

Figure S14. Example tab-delimited user-specified peridotite/harzburgite constant partition coefficient input file containing a header row and non-numeric first column. This file structure is readily input into *REEBOX PRO*.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
1	0.00018	0.0003	0.00001	0.0004	0.005	0.0005	0.00002	0.0004	0.0005	0.00001	0.001	0.00019	0.001	0.001	0.01	0.005	0.002	0.02	0.002	0.002	0.005	0.002	0.0015	0.0015
2	0.006	0.0006	0.001	0	0.0031	0.004	0.0001	0.002	0.003	0.0013	0.0048	0.007	0.0068	0.01	0.01	0.01	0.013	0.024	0.016	0.022	0.028	0.03	0.049	0.06
3	0.0007	0.0007	0.00068	0.0008	0.0077	0.01	0.001	0.0536	0.0858	0.01	0.1	0.13	0.19	0.29	0.12	0.26	0.47	0.38	0.48	0.44	0.4	0.39	0.43	0.43
4	0	0	0.0024	0.012	0.086	0.08	0	0.0012	0.0019	0	0.0023	0.003	0.01	0.007	0.56	0.65	0.01	0.048	0.016	0.01	0.05	0.01	0.01	0.28
5	0.007	0.0007	0.0007	0.005	0.02	0.015	0.013	0.01	0.021	0.0005	0.045	0.006	0.087	0.217	0.32	0.32	0.4	0.2	0.498	1.06	2.11	3	4.03	5.5

Figure S15. Example tab-delimited user-specified peridotite/harzburgite constant partition coefficient input file containing no header row or non-numeric first column. This file structure is readily input into *REEBOX PRO*.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1		Rb	Ba	Th	U	Nb	Ta	K	La	Ce	Pb	Pr	Sr	Nd	Sm	Zr	Hf	Eu	Ti	Gd	Dy	Y	Er	Yb	Lu
2	clinopyroxene	0.0018	0.006	0.0032	0.0041	0.005	0.011	0.03	0.027	0.055	0.042	0.11	0.067	0.122	0.19	0.1	0.22	0.179	0.38	0.318	0.42	0.47	0.51	0.55	0.56
3	garnet	0.005	0.005	0.0008	0.0045	0.005	0.004	0	0.012	0.005	0.056	0.011	0.01	0.057	0.19	0.19	0.22	0.208	0.25	0.584	1.72	2.62	3.42	5.71	7.03

Figure S16. Example tab-delimited user-specified pyroxenite constant partition coefficient input file containing a header row and non-numeric first column. This file structure is readily input into **REEBOX PRO**.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
1	0.0018	0.006	0.0032	0.0041	0.005	0.011	0.03	0.027	0.055	0.042	0.11	0.067	0.122	0.19	0.1	0.22	0.179	0.38	0.318	0.42	0.47	0.51	0.55	0.56
2	0.005	0.005	0.0008	0.0045	0.005	0.004	0	0.012	0.005	0.056	0.011	0.01	0.057	0.19	0.19	0.22	0.208	0.25	0.584	1.72	2.62	3.42	5.71	7.03

Figure S17. Example tab-delimited user-specified pyroxenite constant partition coefficient input file containing no header row or non-numeric first column. This file structure is readily input into **REEBOX PRO**.

Text S4. Model Output File Structure

Output files from REEBOX PRO all have the same general structure. The top portion of the output file contains all of the model input values under the **MODEL INPUTS** header. The bottom portion of the output file contains all of the model output values under the **MODEL OUTPUTS** header. The output files generated for the Standard (Langmuir) RMC and Active (Langmuir) RMC mixing functions have the exact same output structure (although the output model melt compositions differ due to the difference in mixing function). Because the Active (Brown & Leshner) RMC mixing function requires calculation of the net source buoyancy and depends upon the viscosity of the mantle source, additional model inputs and outputs are included in output files generated by this mixing function. The specific similarities and differences are described below.

S4.1. Standard (Langmuir) RMC and Active (Langmuir) RMC Output File Structure

Examples of an output file generated using the Standard (Langmuir) RMC mixing function ('STANDARD RMC BULK CRUST.txt') are shown in Figure S18 (model inputs) and Figure S19 (model outputs). As noted above, the Active (Langmuir) RMC mixing function will generate output files with the exact same output file structure. As shown in Figure S18, the **MODEL INPUTS** portion of the output file contains the model *Source Characteristics* (outlined in red), which contains the specified potential temperature of the mantle adiabat, the initial mass fractions of each lithology (Φ_i^0 ; in this example, the model source contains 10% each hydrous peridotite, harzburgite, G2 pyroxenite, and MIX1G pyroxenite), and the type of peridotite (pyrolite or DMM) for the anhydrous and hydrous peridotite sources.

Below this section is the *Thermodynamic Variables* section (outlined in blue in Figure S18), which contains the isobaric specific heat capacity (Cp), coefficient of thermal expansion (α_S), the entropy of melting (dS) for each of the lithologies, and the density of basaltic melt (rho_melt). Below the *Thermodynamic Variables* section is the *Initial Source Composition(s)* section (outlined in green in Figure S18). For the "BULK CRUST" output file in the main output folder, this section contains the initial trace element and isotopic composition for *each* source lithology (and the initial water content for the hydrous peridotite lithology). Because all other output files (i.e. those files found in the Instant_Melts, Col_Accum_Melts, and Pooled_Melts folders) are specific to each source lithology, the *Initial*

Source Composition section in these other output files will contain the initial composition of that lithology only (Figure S20). For **all** output files, the model inputs pertaining to any pre-existing lithosphere, including the density of continental crust (rho_CC), density of lithospheric mantle (rho_LM) and the fraction of continental crust in the lithosphere (f_crust) are located below the *Initial Source Composition(s)* section (outlined in orange in Figure S18).

In **all** output files generated for the Standard (Langmuir) RMC and Active (Langmuir) RMC mixing functions, the **MODEL OUTPUTS** section *always* begins with the properties of the bulk crust (*Bulk crust properties* section) calculated using the specified mixing function (outlined in red in Figure S19). These bulk crust properties include the igneous crustal thickness (Crust), the pressure at the base of the crust+lithosphere, the proportion of crust derived from the melts of each lithology (X_per_dry, X_per_wet, X_harz, X_G2, X_MIX1G), and the modeled pooled melt composition (in ppm), bulk water content, and mean isotopic compositions of the bulk crust.

compositions of that lithology, depending on the type of output file selected. Figure S20 shows an example of the output file containing instantaneous melt compositions of G2 pyroxenite, calculated using the Standard (Langmuir) RMC mixing function.

S4.2. Active (Brown & Lesher) RMC Output File Structure

The output files generated for the Active (Brown & Lesher) RMC mixing function are very similar to those generated for the Standard (Langmuir) RMC and Active (Langmuir) RMC mixing functions, with the exception of minor differences in the model input and model output sections. Because the Brown and Lesher mixing function calculates mantle flow as a function of source buoyancy, additional model inputs such as ambient mantle potential temperature, half-spreading rate, and mantle viscosity become important. As shown in Figure S20 for the 'BROWN_LESHER RMC BULK CRUST.txt' output file, in addition to the model inputs listed for the Standard (Langmuir) RMC and Active (Langmuir) RMC mixing functions, the MODEL INPUTS section for the Active (Brown & Lesher) RMC mixing function include ambient mantle potential temperature (outlined in red), plate half-spreading rate (outlined in green), and mantle viscosity parameters (outlined in blue). Given that the net source buoyancy and mantle flow are calculated using the Brown & Lesher mixing function, the MODEL OUTPUTS section includes a *Mantle Flow Parameters* section (outlined in orange in Figure S21). This *Mantle Flow Parameters* section outputs the net source buoyancy ($\Delta\rho$) calculated at either the deepest solidus or base of the buoyant flow layer (whichever is deeper), the buoyancy flux (B), the viscosity at the deepest solidus or base of the buoyant flow layer (whichever is deeper), the radius of buoyant flow (R_{flow}), the thickness of the buoyant flow layer (H_{flow}), the total mean upwelling velocity, and the total mean upwelling velocity normalized by the half-spreading rate (γ).

Because the Active (Brown & Lesher) RMC mixing function requires iterative calculations to quantify the thickness of igneous crust generated, the MODEL OUTPUTS section includes how well the iterative calculations converged on the igneous crustal thickness (a small number means excellent convergence), as highlighted in purple in Figure S21. Finally, because the horizontal flow varies as a function of depth with the Active (Brown & Lesher) RMC mixing function, the MODEL OUTPUTS include the pressure dependent horizontal flow normalized by the half-spreading rate ($U(P)$) as outlined in pink in Figure S21. The additions described above are also included in all of the other output files (e.g.

instantaneous, column-accumulated, and pooled melt output files) generated for the Active (Brown & Lesher) RMC mixing function.

The screenshot shows a detailed spreadsheet with the following sections and highlighted areas:

- MODEL INPUTS:**
 - Source characteristics: Tpot (C) = 1340 (highlighted in red).
 - Thermodynamic Variables: alpha_5 (1/K) = 3.00E-05 (highlighted in green).
 - Initial Source Composition: Various trace elements like Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Ti, Gd.
 - pre-existing lithosphere: half-spreading rate (cm/yr) = 1.5 (highlighted in green).
 - Lithosphere Density Variables: rho_CC (kg/m³) = 0 (highlighted in blue).
 - Marine Viscosity Variables: E_act (J/mol) = 1.90E+05, V_act (m³/mol) = 4.00E-06, P_ref (GPa) = 6.75 (highlighted in blue).
 - Marine Flow Parameters: B (kg/s) = 5.36, viscosity (Pa-s) = 88.6, R_flow (km) = 1.24E+19, H_flow (km) = 56, total mean upwelling velocity gamma = 116.92, 6.77 (highlighted in orange).
- MODEL OUTPUTS:**
 - Crust (km) = 52.62 (highlighted in purple).
 - Convergence difference (km) = 4.18E-05 (highlighted in purple).
- MODEL RESULTS:**
 - Final Pooled Melt Composition at Each Decompression Step: A table with columns for elements (Rb, Ba, Th, U, Nb, Ta, K, La, Ce, Pb, Pr, Sr, Nd, Sm, Zr, Hf, Eu, Ti, Gd) and rows for different stages (X_per_dry, X_per_wet, X_harz, X_G2, X_MIXIG).

Figure S21. Example model output file ('BROWN_LESHER RMC BULK CRUST.txt') generated using the Active (Brown & Lesher) RMC mixing function. Additional information included in this output file that is not included in the Standard (Langmuir) RMC or Active (Langmuir) RMC output files is outlined in red, green, blue, orange, purple, and pink.

Text S5. Worked Examples

To illustrate the use of **REEBOX PRO**, the sections below provide two worked examples. The first example runs a melting calculation for a source consisting solely of anhydrous peridotite, using the Standard (Langmuir) RMC mixing function. The second example runs a melting calculation for a heterogeneous source containing hydrous peridotite, harzburgite, and G2 pyroxenite, using the Active (Brown & Lesher) RMC mixing function.

55.1. Homogeneous Source, Standard (Langmuir) RMC Mixing Function

In this first example, we illustrate the simplest modeling scenario- melting of a homogeneous source consisting entirely of anhydrous peridotite using the Standard (Langmuir) RMC mixing function and no pre-existing lithosphere. In this example, we will use the default isotopic compositions. The only things that need to be specified are the type of peridotite (pyrolite or DMM), the initial trace element composition of the peridotite source

(both in the *Source Lithology Input* → *Anhydrous Peridotite* section) and the potential temperature of the mantle adiabat (*Other Inputs* → *Conditions For Model Run* section). For this example, select *pyrolite* for the peridotite type, *Primitive Mantle (McDonough & Sun 1995)* for the initial trace element composition, and 1440 °C for the *Mantle Potential Temperature*. Now, click the *Run Calculation* button to execute the model calculation. Once the model finishes, you should see that the model results in 14.72 km thick igneous crust (in the *Messages* section). Click the *Save Results* button, navigate to the directory where you'd like to keep the output file, and save the output files. Navigate to that location on your hard drive, and open the files in Excel (or other spreadsheet program) to begin familiarizing yourself with the output files (see **Text S4**).

55.2. Heterogeneous Source, Active (Brown & Lesher) RMC Mixing Function

For a slightly more complex modeling scenario, we now consider melting of a lithologically heterogeneous mantle source containing hydrous peridotite (DMM), non-melting harzburgite, and G2 pyroxenite, using the Active (Brown & Lesher) RMC mixing function and assuming a half-spreading rate of 2 cm/yr and a pre-existing lithospheric thickness of 40 km. To begin, use the *Model Reset* menu to reset all model parameters to their default values. For this example, we will use the following source abundances: 80% hydrous peridotite, 5% harzburgite, 15% G2 pyroxenite. Enter these values into the appropriate *Initial Source Abundance (%)* input boxes. For the hydrous peridotite source, set the peridotite type to *DMM*, the initial water content to 150 ppm, and select *DMM (Salters & Stracke 2004)* for the initial trace element composition. Change the initial isotopic compositions for the hydrous peridotite source to $87\text{Sr}/86\text{Sr} = 0.702460$, $143\text{Nd}/144\text{Nd} = 0.513200$, $176\text{Hf}/177\text{Hf} = 0.283100$, and $206\text{Pb}/204\text{Pb} = 17.750$. For harzburgite, uncheck the *harzburgite melts* box (we do not want harzburgite to melt in this example), which should result in the compositional input boxes for harzburgite becoming inactive. For G2 pyroxenite, select *NMORB (Sun & McDonough 1989)* for the initial trace element composition, and use the default initial isotopic compositions. Change the *Half-Spreading Rate* to 2 cm/yr, and the *Pre-Existing Lithosphere* to 40 km (both are located in the *Other Inputs* → *Conditions For Model Run* section).

Because the default mantle potential temperature is 1330 °C, you should see that presently the net source buoyancy is -13.96 kg/m³ (at the bottom of the *Other Inputs* → *Ambient Mantle* section). Because the Active (Brown & Lesher) RMC mixing function requires

positive net source buoyancy, we will need to create a thermal anomaly to offset the negative compositional buoyancy. To do this, we will create a 200 °C thermal anomaly. First, uncheck the *Use Mantle Potential Temperature* box in the *Other Inputs* → *Ambient Mantle* section. Now, change the Mantle Potential Temperature (located in the *Other Inputs* → *Conditions For Model Run* section) to 1530 °C. You should now see that the net source buoyancy is now 4.35 kg/m³. To finish, select the Active (Brown & Lesher) RMC mixing function (located in *Other Inputs* → *Mixing Function* section), and click the *Run Calculation* button. Once the model is completed, you should see that the Standard (Langmuir) RMC mixing function would generate an igneous crustal thickness of 17.42 km, whereas the Brown & Lesher mixing function generates a crustal thickness of 19.7 km. Again, to familiarize yourself with the model output files, click the *Save Results* button and save the output files to your hard disk (see **Text S4**).

55.3. REEBOX PRO Batch Run

At present, the stand-alone version of **REEBOX PRO** is not configured to process batch runs (e.g. exploring parameter space over wide ranges of potential temperatures and initial lithologic abundances). However, if you are interested in using **REEBOX PRO** in such a manner, please contact Eric Brown (ericlb@geo.au.dk) about the possibilities.

Supporting References

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Langmuir, C. H., Klein, E. M., and Plank, T. (1992), Petrological systematics of mid-ocean ridge basalts: Constraints on melt generation beneath ocean ridges, in *Mantle Flow and Melt Generation at Mid-Ocean Ridges, Geophysical Monograph Series, 71*, edited by J. Phipps Morgan et al., p. 183-280, AGU, Washington, D.C.