Energy-Constrained Recharge, Assimilation, Fractional Crystallization (EC-RAχFC): A Visual Basic Computer Code for Calculating Trace Element and Isotope Characteristics of Open-System Magmatic Systems

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Abstract: Volcanic and plutonic rocks provide abundant evidence for complex processes that occur in magma chambers and as magma travels from source to surface. The fingerprint of these processes, which include fractional crystallization, assimilation, and magma recharge, is captured in petrologic and geochemical characteristics of suites of cogenetic rocks. Quantitatively evaluating the relative contributions of each process requires integration of mass, species and energy constraints, applied in a self-consistent way to conservation equations. The energy-constrained model EC-RAχFC (Energy-Constrained Recharge, Assimilation and Fractional Crystallization) tracks the trace element and isotopic evolution of a magmatic system (melt + solids) undergoing simultaneous fractional crystallization, recharge and assimilation. Mass, thermal, and compositional (trace element and isotope) output are provided for melt in the magma chamber, cumulates, enclaves, and anatectic melt. Theory of the EC computational method has been presented in Spera and Bohrson, 2001, 2002, 2004 and applications to natural systems have been elucidated in Bohrson and Spera, 2001, 2003 and Fowler et al. 2004. The purpose of this contribution is to make the final version of the EC-RAχFC computer code available, as well as provide instructions for code implementation, description of input and output parameters, and estimates of typical values for some input parameters. A brief discussion highlights measures by which the user may evaluate the quality of the output. The EC-RAχFC computer code is written in Visual Basic, the programming language of Excel. The code therefore launches in Excel and is compatible with both PC and MAC platforms. The code is available on a number of websites (e.g., http://magma.geol.ucsb.edu/, http://www.geology.cwu.edu/ecrafc).

Keywords: EC-RAχFC, energy-constrained, assimilation, recharge, mass balance, magma chamber

1. Introduction

The compositional diversity of igneous rocks on Earth results from a complex array of processes, many of which occur in magma reservoirs or during vertical or lateral transport within conduits. Elemental and isotopic data collected at a variety of scales during the last several decades indicate that first-order magma chamber processes include magma recharge, country rock assimilation, and fractional crystallization (RAFC). Several quantitative models have been developed that predict the geochemical paths of magmas that undergo RAFC [e.g., O'Hara, 1977; O'Hara and Mathews, 1981; Albarede, 1995; DePaolo, 1985], and application of these models has led to an increasingly sophisticated understanding of magmatic processes. The approach we have taken, which is to self-consistently couple energy, mass and species conservation, has led to the development of the energy-constrained model EC-RAχFC (Energy-Constrained Recharge, Assimilation and Fractional Crystallization). EC-RAχFC tracks the trace element and isotopic evolution of a magmatic system (melt + solids) simultaneously undergoing fractional crystallization, recharge and assimilation. The theoretical underpinnings of the EC approach have been detailed in a number of publications [Spera and Bohrson, 2001, 2002, 2004] and applications to natural systems have also been proffered [Bohrson and Spera, 2001, 2003; Fowler et al., 2004]. EC-RAχFC is presented as a visual basic computer code, the programming language of Excel, and is compatible with both MAC and PC platforms. Our purpose here is to provide instructions to the user for implementation of the code, including explanation of the input and output. We also provide a brief description of criteria by which the user can judge the quality of model output.

2. Model Overview

In EC-RAχFC, a composite magmatic system (Figure 1) is envisioned that is isolated adiabatically from its environment. The composite system comprises three sub-systems: the magma body, the country rock, and a reservoir of recharge magma. The boundaries between these sub-systems may be open, closed or semi-permeable with respect to mass and adiabatic or diathermal with respect to energy. Country rock is separated from the magma body by diathermal, semi-permeable boundaries. That is, heat can freely pass across a boundary that is permeable to fraction χ of anatectic melt generated in the country rock by partial fusion. An additional sub-system includes a reservoir of recharge melt of arbitrary mass, specific enthalpy (or temperature) and composition. During episodes of recharge, the boundary between the recharge reservoir and the magma body is open with respect to matter and heat. The magma body consists of host melt, cumulates, and enclaves. Cumulates are those solids that fractionate from the host melt, whereas enclaves form by crystal fractionation of unmixed recharge melt when recharge is intruded into the magma body at a temperature greater than that of the local magma temperature.

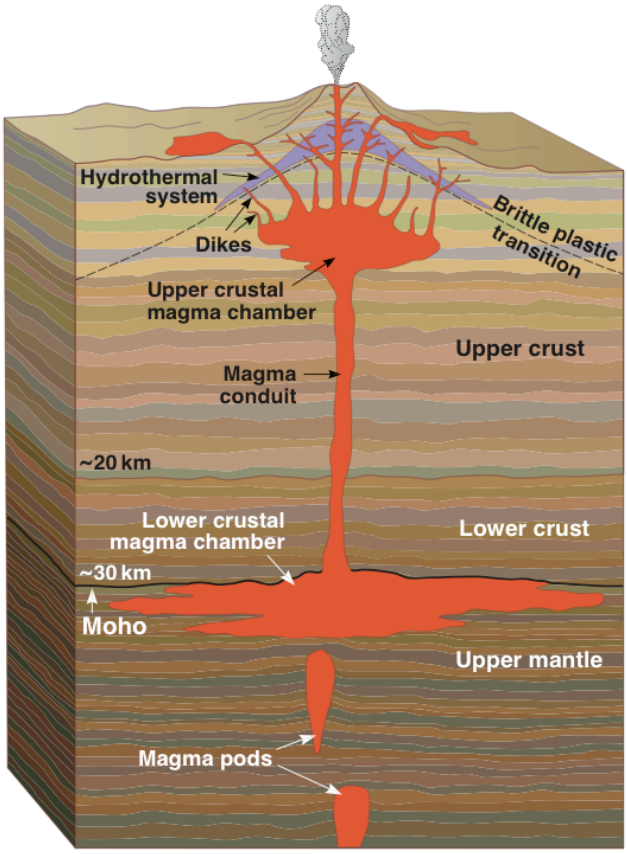

Figure 1: Schematic illustration of the composite magmatic system depicted in EC-RAχFC code. A body of magma (sub-system 1, upper crustal magma chamber) resides in the crust (sub-system 2, upper crust). The magma body may be affected by input from below via a reservoir of recharge magma (sub-system 3, lower crustal magma chamber). Mass and energy are transported between the sub-systems according to assumptions of the energy-constrained model.

The critical aspect of EC-RAχFC is that enthalpy transport from magma to country rock leads to formation cumulates in the magma chamber. This enthalpy loss, which is due to both magma cooling and crystallization, will heat country rock and induce anatexis when the country rock temperature exceeds the local solidus. Additional enthalpy delivered by recharge magma will also impact the amount of energy available to heat and potentially melt country rock. The degree of melting experienced by country rock depends on its fraction of melt-temperature relationship –the so-called melt productivity function—and the amount of heat provided by magma (±recharge) cooling and crystallization. The fraction of anatectic melt delivered to the magma body is governed by the user-chosen parameter χ (labeled as X in the code) which is defined as the mass of anatectic melt delivered to the magma body relative to the amount (mass) of anatectic melt generated ($0 \leq \chi \leq 1$). Upon addition of anatectic or recharge melt, melt in the magma body is efficiently homogenized. Chemical changes in the magma body are modeled by fractional crystallization, with appropriate variation as a result of recharge and assimilation. Enclave formation (the instantaneous freezing of a portion of recharge melt) from recharge magma is also modeled by fractional crystallization. Melting in country rock is modeled as a fractional process.

By solving expressions describing conservation of enthalpy, mass, trace species, and isotopic ratios, the code computes changes in the compositions, thermal characteristics, and masses of melt and solids as each sub-system approaches a state of thermal equilibrium. More specifically, EC-RAχFC is formulated as a set of $3+t+i+s$ coupled nonlinear differential equations, where the number of trace elements, radiogenic and stable isotope ratios modeled are t, i and s,

131 respectively. The independent variable is conveniently taken as the temperature of melt (T_m)
132 within the magma body. Each numerical simulation is run until all sub-systems reach a common
133 equilibration temperature defined by the user. For derivation of all equations, discussion of
134 assumptions and other relevant issues, the reader is referred to Spera and Bohrson [2001, 2002,
135 2004] and Bohrson and Spera [2001, 2003].
136

137 ## 3. Implementation

138 In this section, we provide a description of the computer code, instructions for implementation,
139 description of input and output parameters, and estimates of typical values for some input
140 parameters.
141

142 ### *3.1 Description of Computer Code*

143 The computer code is written in visual basic, the programming language of Excel. The code
144 therefore launches in Excel and is compatible with both PC and MAC platforms. Code
145 calculations are broadly divided into two parts: the first is an integral calculation that determines
146 the total enthalpy balance for the entire system, given a set of thermal and other parameters for
147 all sub-systems. The output from this calculation is a set of ordered pairs that include the
148 equilibration temperature and the total mass of country rock that comes into thermal equilibrium
149 with the magma body (±recharge magma). The second involves path-dependent calculations that
150 rely on solutions to $3+t+i+s$ differential equations, which are solved numerically using a fourth
151 order Runge-Kutta method. The user chooses one equilibration temperature, based on knowledge
152 of the thermal environment (see evaluation in Spera and Bohrson, 2001), and also defines the
153 relevant compositional parameters and the mass of recharge-magma temperature function. Path-

dependent calculations are computed, yielding thermal, chemical, and mass information about the sub-systems. Because the progress variable is the temperature of the magma, the path is defined by a series of temperature steps, the size of which is chosen by user.

3.2 Access and Instructions for Executing the Code

The EC code can be downloaded from the following websites: http://magma.geol.ucsb.edu/, http://www.geology.cwu.edu/ecrafc, http://www.petrology.oxfordjournals.org, and http://earthref.org/GERM/index.html?main.htm.

To execute the code, double click on the icon and click "enable macros." The main menu page will appear. Maneuvering between pages in the code happens simply by clicking the relevant button. The user is first required to set input parameters for the integral calculation (Part 1). At the conclusion of this calculation, a menu of paired values of equilibration temperature and mass of wallrock appears. The user chooses one pair, and then sets parameters for the path-dependent calculation. Output for the path-dependent calculation appears as two pages, one that tracks melt and one that tracks solids. Each output sheet is stored as a labeled worksheet and is accessible via worksheet tabs at the bottom of the Excel file. The user also has the option of evaluating results from standard graphical output and can also customize graphing options. A **Help button** provides some basic information about the code; a more detailed documentation file (ECRAXFC.help.pdf) is also available. Note that EC-RAχFC and EC-RAXFC are equivalent.

3.3 Part 1 Integral Energy Calculation: Input and Output

The user is required to enter input in five categories, which appear as buttons at the top of the Excel file: Thermal, Melting Functions, Recharge, X, Initial Conditions. Note that χ and X are equivalent, and assimilant and wallrock are used synonymously.

Below is Table 1, which describes thermal input parameters **(Thermal button)**, and provides typical ranges of values of basaltic to silicic composition magmas. Pristine magma refers to melt in the magma body at the start of the simulation, before any anatectic melt or recharge melt has been added to the chamber. The user is required to enter values for all of the parameters that are relevant to the simulation.

Mass parameters in the code are nondimensional and are relative to the mass of melt in the magma chamber at the start of the simulation (M_m^o). Thus, the initial condition for the magma chamber is a nondimensional mass ($\overline{M}_m^o$) of 1. A nondimensional mass for country rock ($\overline{M}_a^o$) or total mass of recharge ($\overline{M}_r^o$) of 3 indicates that the wallrock or recharge mass involved in the simulation is three times that of the magma chamber at the start of the simulation. In some cases, nondimensional temperatures are also reported in the code, which are relative to the initial temperature of the magma body ($\overline{T}_m = \frac{T_m}{T_m^o}$). Although sometimes reported in centigrade, all computations involving temperature are carried out using the SI unit of temperature (Kelvin).

199 Table 1: Explanation of Thermal Input Parameters for Part 1 Integral Calculation

Label in code	**Explanation**	**Typical Range basaltic → silicic**	**Units**
tlm	liquidus temperature of pristine magma	1200-950	°C
tmo	initial temperature of pristine magma	1200-950	°C
tla	liquidus temperature of assimilant (country rock)	1200-950	°C
tao	initial temperature of assimilant	250-600	°C
tlr	liquidus temperature of recharge	1200-1000	°C
tro	initial temperature of recharge magma. Default setting is equal to tlr	1300-1000	°C
ts	solidus, common to pristine magma, assimilant, and recharge magma	900	°C
cpm	specific heat, pristine magma	1000-1200	J/ kg K
cpa	specific heat, assimilant	900-1100	J/ kg K
cpr	specific heat, recharge magma	1000-1200	J/ kg K
hm	heat of crystallization, pristine magma	350000-500000	J/kg
ha	heat of fusion, for assimilant	250000-450000	J/kg
hr	heat of crystallization, recharge magma	350000-500000	J/kg

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201 The Linear and Non-Linear Crystallization and Melting page (**Melting Functions button**)
202 allows a choice of melting/crystallization productivity functions, which prescribe the relationship
203 between temperature and mass fraction of melt. Although linear productivity functions can be

used, we recommend that the user choose non-linear logistical parameters because they more accurately reflect how rocks melt or magmas crystallize. For non-linear logistical, two parameters, 'a' and 'b' characterize melt productivity curves for pristine magma, assimilant and recharge magma. A full discussion of the significance of these parameters is given in section 4.2 of Spera and Bohrson [2002]. The user chooses the parameters 'a' and 'b' to match an assumed melt productivity relationship. Typical ranges for 'a' and 'b' are 400 to 450, and –11 to –13, respectively. In practice, one might have access to experimental data or run a MELTS (Ghiorso and Sack, 1995) simulation to develop the melt fraction vs. temperature relationship. Then, for a given liquidus temperature and solidus temperature, the parameters 'a' and 'b' are adjusted to capture the melting curves. A graphical display of the fraction of melt vs. temperature is provided in the code. In order to examine this plot, click the **View Non Linear Melt Chart button**. Typically one must find the 'a' and 'b' parameters by trial and error interaction. Use of the graphical output makes it rather straightforward; after a few tries, one can intuitively access the sensitivity of the melt productivity functions for pristine magma, recharge and country rock on the parameters 'a' and 'b'.

The recharge parameters page **(Recharge button)** requires the user to enter the total nondimensional mass of recharge magma. For example, a nondimensional mass of recharge magma of 0.5 means that during the simulation, the total mass of recharge material that enters the magma chamber is half of the mass of the magma chamber at the start of the simulation. Note that the temperature-recharge mass relationship is set in Part 2; that is, the temperature of the magma, T_m at the moment recharge magma is added to the magma body is set in Part 2 of the calculation.

The X page **(X button)** allows the user to set X, the fraction of anatectic melt that enters the magma chamber, relative to the amount generated. X = 0 indicates that no anatectic melt generated enters the chamber, whereas X = 1 means that all anatectic melt generated enters the chamber. In cases where X < 1 it is important to note that energy conservation requires that the appropriate mass of anatectic melt be made, but not all of it is mixed into the magma body; the amount that is not mixed into the magma body remains as part of the country rock sub-system.

The final page for the Part 1 calculation **(Initial Conditions button)** requires the user to input the nondimensional temperature step, which is the size of the nondimensional magma temperature decrement used in the integral calculation. Typical values of this parameter range from –0.001 to –0.0001. All other parameters are set automatically and relevant cells are locked; the user cannot modify these.

The **Run Equilibration button** yields n ordered pairs of T_{eq} (equilibration temperature)- $\overline{M}_a^o$ (total mass of country rock involved in the simulation); these ordered pairs appear on the main menu page in a drop-down menu. Output for Part 1 is stored on the Equilibration worksheet, and results can be accessed by clicking the **View Equilibration Results button**. Below is a table describing parameters listed in this worksheet.

250 Table 2: Explanation of Output for Part 1, Integral Energy Balance Calculation: Equilibration

251 Parameters for EC-RAXFC Simulation

Abbreviation	Explanation
Norm Teq	nondimensional equilibration temperature of system
Teq deg C	equilibration temperature of system, °C
Mm	nondimensional mass of melt in magma body
Mao	nondimensional mass of country rock
Ma*	nondimensional mass of anatectic melt
Intermediate	Cells used in subsequent calculations
Ms	nondimensional mass of all solids (cumulate + enclave)
fa	melt-temperature relationship for country rock (country rock melt productivity function)
fm	crystallization-temperature relationship for pristine magma (magma crystallization productivity function)
fr	crystallization-temperature relationship for recharge magma (recharge magma crystallization productivity function)

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253 ***3.4 Part 2 Path-Dependent Calculation: Input and Output***

254 To execute the path-dependent calculations, the user is required to choose one ordered pair

255 (equilibration temperature (T_{eq})- total mass of wall rock sub-system (M_a^o)) from the available

256 menu. The user is then required to enter path dependent parameters, of which there are 5

257 categories: Isotopes, Trace Elements, Oxygen isotopes, Recharge, and Initial Conditions.

258

Up to three trace element/isotope systems can be entered **(Isotopes button)**. Required information includes element name, concentration in pristine magma, bulk distribution coefficient (D_m^o), and enthalpy. The enthalpy is a measure of the temperature dependence of the partition coefficient. Similar values are required for country rock and recharge magma. A non-zero enthalpy permits the bulk partition coefficient to change as a function of temperature (magma, country rock or recharge magma). For the relevant equations and discussion of this temperature dependence, see Spera and Bohrson [2001]. The most efficient method of choosing an enthalpy (which can be either negative or positive) is to create a spreadsheet that provides solutions to the equations for a range of bulk distribution coefficients over a range of temperatures. By iterating, the user can identify a reasonable range of bulk distribution coefficients for a single simulation. The user is also required to enter the isotope system name (e.g., $^{87}Sr/^{86}Sr$) and the isotope ratios of pristine magma, country rock, and recharge magma. The **Reset button** clears all values from the relevant cells. Three additional trace elements **(Trace Elements button)** can be involved in the calculation, and input data are similar to those required for the isotopes page.

The user has the choice of including oxygen isotopes in the calculation **(Oxygen Isotopes button)**. The $^{18}O/^{16}O$ for pristine magma, country rock, and recharge magma are required. Oxygen concentrations are set by the code for typical values of magma and crust. The user can change these values by clicking the **Unlock button**.

The recharge parameters page **(Recharge button)** requires the user to enter the relationship between the mass of recharge magma entering the magma body and magma temperature. Two

broad choices are provided: linear, which is considered to be a proxy for continuous recharge, and episodic. If episodic is chosen, the user can choose to divide the total nondimensional mass of recharge magma into 1 to 20 pulses (i). For *i* pulses, $\Delta M_{r,i}$ is the mass increment of recharge for pulse 1, 2, to i. $T_{m,i}$ degC is the temperature in °C of the mid-point of the pulse, and $m_{r,i}$ and d_i define the steepness and inflection location of the curve. The sum of $\Delta M_{r,i}$ (all episodes) tracks the total $M_{r,i}$ entered by the user for all pulses and must equal M_r^o. To view the shape of the recharge-temperature curve, click the **View Recharge Event button**. Information about thermal parameters is echoed on the page to help the user recall thermal parameters that are relevant to setting recharge parameters.

When defining the relationship between the mass of recharge magma entering the magma body and magma temperature, it is critical to ensure that at T_{eq}, the entire mass of recharge magma has entered the magma body. Incomplete addition results from choosing to add $\Delta M_{r,i}$ at a $T_{m,i}$ that is close to T_{eq}. Careful examination of the recharge mass-temperature curve using the **View Recharge Event button** will allow the user to identify cases in which this is the case.

The initial conditions page **(Initial Conditions button)** requires three actions. The first is the choice of deltaT, which is the nondimensional temperature step used as the progress variable. Typical values for reconnaissance calculations are –0.001 to –0.0005. However, smaller steps (as small as- 0.00001 in rare cases) may be required under certain conditions and/or for a detailed understanding of the chemical evolution of a magmatic system. When one has arrived at what seems to be a good solution, the fail-safe test is to drop the deltaT again by a factor of 5-10 and re-run the simulation. Although it may take a few minutes, the solution should be essentially

identical to the previous one if the previous deltaT was sufficiently small. Additional details about deltaT are provided in the discussion section. The user also has the option of naming the output worksheets, and can choose to turn on/off the graphing capabilities. Additional cells, which are labeled, show particular values that are relevant to the Run Path Dependent calculations; these cells are locked and therefore, the user does not have the option of modifying values in these cells.

Run Path Dependent yields two pages of numerical output and an additional page of associated graphs, if the graphing function is active. Both numerical output pages echo the input parameters for the simulation. The first page provides output mostly relevant to melt in the magma body. Below, Table 3 provides an explanation of the melt output parameters.

Table 3: Explanation of Output for Part 2, Path-Dependent Calculation, Melt: EC-RAXFC Results—Melts Page

Abbreviation	Explanation
Norm T magma	normalized magma body temperature
T magma (deg C)	magma body temperature, degrees C[1]
Norm T assim	normalized country rock temperature
T assim (deg C)	country rock temperature, degrees C[2]
Mm	nondimensional mass of melt in magma body
fa	melt productivity function for country rock evaluated at Ta
Ma*	nondimensional mass of anatectic melt generated between Tao and Ta

XMa*	nondimensional mass of anatectic melt added to magma body between Tao and Ta
fm	melt productivity function for pristine magma evaluated at Tm
Mc	nondimensional mass of cumulates formed between Tmo, Tro and Tm (includes contribution that recharge magma makes to mass of cumulates)
Men	nondimensional mass of enclaves formed between Tmo, Tro and Tm
Ms	nondimensional mass of cumulates and enclaves (total solids) formed between Tmo, Tro, and Tm
fr	melt productivity function for recharge magma evaluated at Tm
Mr	nondimensional mass of recharge magma added between start of simulation and Tm
Sr^3	elemental concentration of Sr at this T step
$87Sr/86Sr^3$	isotope value at this T step

[1]T magma is local temperature of magma body on the path to thermal equilibration.

[2]T assim is the local temperature of country rock on the path to thermal equilibration.

[3]Output for trace elements and isotopes will vary, depending on input. If enthalpy values are non-zero, value of bulk distribution coefficient is also output.

The **Add Extra Charts button** allows the user to choose up to 6 additional binary plots. Choices for the x-axis and y-axis are available from a drop-down menu.

The solids output page tracks the masses of enclaves, cumulates, and total solids in two ways; incremental values represent the nondimensional mass of solid produced in a single temperature step, whereas cumulative mass represents the total nondimensional mass that has been generated from T_m^o and T_m. Compositional information is provided for enclaves, cumulates, total solids, and anatectic melt. Instantaneous composition represents the trace element composition of the increment formed in a single temperature step. Average concentration reflects the average composition for solids formed between T_m^o and T_m and for anatectic melt formed between T_a^o and T_a. Trace element masses for each type of solid and anatectic melt all also provided. Isotope values of cumulates are not reported because they are identical to those of melt in the magma body at each temperature step. Enclave isotopic ratios are always those of the recharge magma, and anatectic melt isotope ratios, prior to melt incorporation into the magma body, are identical to those of the country rock.

Table 4: Explanation of Output for Part 2, Path-Dependent Calculation, Solids and Anatectic Melt: EC-RAXFC Results—Solids Page

Abbreviation	Explanation
Norm T magma	normalized magma body temperature
T magma (deg C)	magma body temperature, degrees C
Norm T assim	normalized country rock temperature
T assim (deg C)	country rock temperature, degrees C
iMen	incremental mass of enclaves (nondimensional)
Men	cumulative mass of enclaves (nondimensional)
Intermediate	These cells are used in subsequent calculations and should be

	ignored
iMc	incremental mass of cumulates (nondimensional)
Mc	cumulative mass of cumulates (nondimensional)
Ms	cumulative mass of solids (cumulates +enclaves) (nondimensional)
iCen [element][1]	instantaneous concentration of trace element in enclaves
Cav,en	average concentration of trace element in enclaves
Mtr,en	mass of trace element in enclaves
iCc	instantaneous concentration of trace element in cumulates
Intermediate	These cells are used in subsequent calculations and should be ignored
Mtr,c	mass of trace element in cumulates (nondimensional)
Intermediate	These cells are used in subsequent calculations and should be ignored
Cav,c	average concentration of trace element in cumulates
Cav,s	average concentration of trace element in solids (cumulates +enclaves)
iCa	instantaneous concentration of trace element in anatectic melt
Cav,a	average concentration of trace element in anatectic melt
Mtr,a	mass of trace element in anatectic melt (nondimensional)
% error, total mass of trace element	Percent error in mass balance of trace element in system[2]

[1]Element name labeled in cell above. Output will vary because for each element, relevant output will be displayed.

[2]Mass balance check is described fully in discussion section.

3.5 Graphing Capabilities

Standard graphical output is an option in the EC code. Magma body temperature is the x-axis value and y-axis values include mass, temperature and compositional output. The user has the choice to tailor additional graphical output using the drop down menus available on the melts output sheet (Add Extra Charts).

4. Discussion

Because the path dependent calculations rely on numerical solution of the coupled non-linear equations representing conservation of energy, mass and species, numerical issues can arise during execution of Part 2 of the code. Coarse deltaT steps (chosen on the Initial Conditions page of Part 2) can potentially result in numerical instability that can be manifested in thermal, mass or compositional parameters. Numerical errors are greater in cases where M_a* or M_r^o is large and/or bulk distribution coefficients are extreme (e.g., $D_m^o = 0.001$). There are several simple tests that the user can apply to ensure that the deltaT step is small enough to generate reliable results.

The first test involves comparing the final magma body temperature T_m (which should be very close to the chosen equilibration temperature) to the final country rock temperature (T_a) on the melt output pages for Part 2. Smaller delta T steps typically will yield closer agreement. For typical conditions with deltaT of –0.0005, the difference between the magma T_{eq} and country rock T_{eq} will be less than a few °C. Similar comparisons can be made for the final values of

masses (e.g., M_m, M_c, M_{en}); these final values should be close to those determined in the integral calculation for a particular equilibration temperature. If they are not within a few percent of the integral values, the temperature decrement should be made smaller. Note that integral values for many of these parameters are echoed on the Melts and Solids output pages.

The user is also referred to the mass balance output on the solids and anatectic melt page. This mass balance is defined by the following equation:

$$1 + \overline{M}_r(\overline{T}_m)C_r^o + \chi\,\overline{M}_a^*(\overline{T}_m)\hat{\overline{C}}_a = \overline{M}_m\overline{C}_m + \overline{M}_{en}\hat{\overline{C}}_{en} + \overline{M}_c\hat{\overline{C}}_c \qquad (1)$$

This expression represents a mass balance for a given trace element. It represents the fact that the total mass of trace element that is initially present plus that which is added by recharge and assimilation must be balanced by the a mass of trace element in the melt plus that locked up in enclaves and cumulates that form during cooling and crystallization. If we let the LHS of (1) be A and the RHS be B, then we can compute a parameter $\left(\frac{A-B}{A}\right)100$. This is precisely the number reported in the solids + anatectic melt output sheet (% error, total mass of trace element). It is the percent error of this mass balance. Typically, the absolute value of this deviation should not exceed 2-3%. If it does, the deltaT step is too large and the user should go back and recompute a path 2 evolution using a smaller temperature decrement.

A third check on the quality of output involves comparing output run at two different deltaT steps, with all other parameters being equal. Differences in path-dependent values, such as trace element concentrations or isotope values that exceed the analytical uncertainty, indicate that the

large deltaT step is too coarse. The user should iterate until two runs with slightly different deltaT steps yield results similar within typical analytical uncertainty. For most cases, convergence of the solutions will happen for deltaT steps of order –0.0005 to –0.0001. Large M_a^*, M_r^o and/or extreme bulk distribution coefficient values may require finer delta T steps.

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