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Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RAχFC): A Visual Basic computer code for calculating trace element and isotope variations of open-system magmatic systems

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[1] Volcanic and plutonic rocks provide abundant evidence for complex processes that occur in magma storage and transport systems. 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. The energy-constrained model Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RaχFC) 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 is provided for melt in the magma body, cumulates, enclaves, and anatectic (i.e., country rock) melt. Theory of the EC computational method has been presented by Spera and Bohrson (2001, 2002, 2004), and applications to natural systems have been elucidated by 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 and to 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 and also provides some guidelines for implementing nonlinear productivity functions. 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 the authors' Web sites http://magma.geol.ucsb.edu/and http://www.geology.cwu.edu/ecrafc) as well as in the auxiliary material.

1. Introduction

[2] 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. For purposes of this work, this system of reservoirs and conduits will be referred to as a magma plumbing system. Elemental and isotopic data collected at a variety of scales during the last several decades indicate that first-order magma plumbing system 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; *Albaréde*, 1995; *DePaolo*, 1981], 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 Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RaχFC). 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]. A previous version of the code was informally released on the authors' and GERM Web sites, although no formal documentation was made available. We note that this older version lacked implementation of the χ function and also lacked output on solids and anatectic melt. In the new version, several additional features are available, including additional graphing functions. *Spera and Bohrson* [2004] implement eruption in the EC approach (i.e., EC-ERAχFC) but also note limitations that restrict application to many natural systems. For this reason, the eruption function is not available with the version of the code discussed in this document. Full implementation of eruption is a subject of ongoing research and will be presented in another computer model (Magma Chamber Simulator [*Bohrson et al.*, 2006]). 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 and discuss how best to approach using the nonlinear productivity functions described below.

2. Model Overview

[3] 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 (sub-system 1), the country rock (sub-system 2), and a reservoir of recharge magma (sub-system 3). (The term *magma body* will be used to describe melt + solids associated with sub-system 1, including any mass added through addition of anatectic melt, recharge melt and enclaves). 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 and added to the magma body. During episodes of recharge, the boundary between the recharge reservoir and the magma body is open with respect to matter and heat; recharge melt and enclaves (defined below) are added to the magma body. The magma body therefore consists of melt (with possible contributions from country rock and recharge reservoir), cumulates, and enclaves. Cumulates are those solids that fractionate from magma body melt, whereas enclaves form by crystal fractionation of unmixed recharge melt when recharge magma is intruded into the magma body at a temperature greater than that of the local magma temperature.
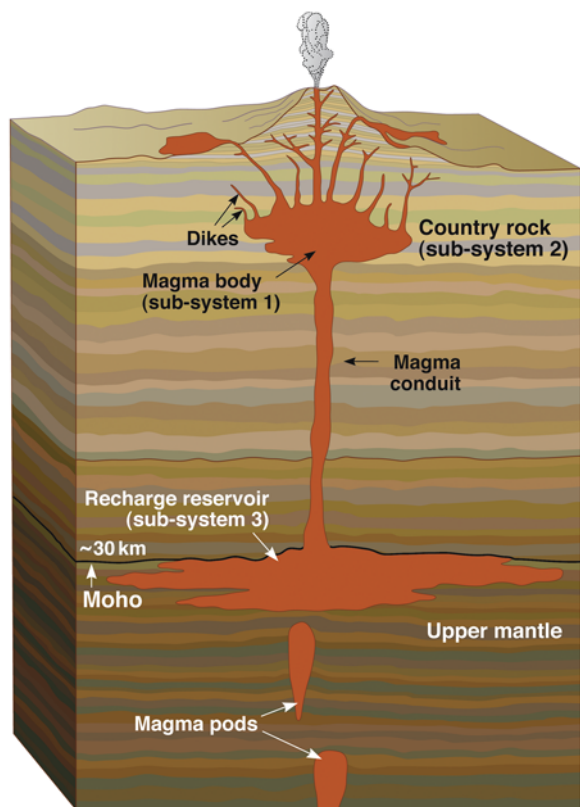
Figure 1. Schematic illustration of the composite magma plumbing system depicted in EC-RAχFC code. A magma body (sub-system 1, shown in the upper crust) is surrounded by country rock (sub-system 2, depicted as upper crust). The magma body may be affected by input from below via a reservoir of recharge magma (sub-system 3, shown in lower crust). Note that the size, shape, and location of the sub-systems and the connecting conduit shown in this illustration are schematic. Different magma plumbing system structures may also be modeled using the EC approach.

[4] The critical aspect of EC-RAχFC is that enthalpy transport from the magma body to country rock leads to formation of cumulates in the magma body. This enthalpy loss from the magma body, which is due to both 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 contribute to the amount of energy available to heat and potentially melt country rock. The degree of melting experienced by country rock depends on the relationship between fraction of melt and temperature, which here is defined as the melt productivity function. 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 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.

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

3. Implementation

[6] This section provides a description of the computer code, instructions for implementation, description of input and output parameters, and estimates of typical values for some input parameters.

3.1. Description of Computer Code

[7] Code calculations are broadly divided into two parts: the first is an integral calculation that determines the total enthalpy balance for the entire system (i.e., all sub-systems), given a set of thermal and other parameters for all sub-systems. The output from this calculation is a set of ordered pairs that include the equilibration temperature and the total mass of country rock that comes into thermal equilibrium with the magma body (±recharge magma). The second involves path-dependent calculations that rely on solutions to $3 + t + i + s$

differential equations, which are solved numerically using a fourth order Runge-Kutta method. The user chooses one equilibration temperature, based on knowledge of the thermal environment (see evaluation by *Spera and Bohrson* [2001]), and also defines the relevant compositional parameters and the mass of recharge-magma body temperature function. Path-dependent calculations yield thermal, chemical, and mass information about the sub-systems. Because the progress variable is the temperature of the magma in sub-system 1, the path is defined by a series of temperature steps, the size of which is chosen by the user.

3.2. Access and Instructions for Executing the Code

[8] The EC code can be downloaded from the authors' Web sites http://magma.geol.ucsb.edu/ and http://www.geology.cwu.edu/ecrafc) as well as from the auxiliary material[1] (see Software S1).

[9] 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 country rock appears. The user chooses one of these pairs, and then sets parameters for the path-dependent calculation. Output for the path-dependent calculation appears as two pages, one that tracks melt composition and mass and one that tracks composition and mass information about solids and anatectic melt. 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

[10] 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 country rock are used synonymously.

[11] Table 1 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. The user is required to enter values for all of the parameters that are relevant to the simulation.

[12] Mass parameters in the code are nondimensional and are relative to the mass of melt in the magma body at the start of the simulation (M_m^o). Thus the initial condition for the magma body is a nondimensional mass ($\overline{M}_m^0$) of 1. (Note that overbar indicates nondimensional parameter). A nondimensional mass for country rock ($\overline{M}_a^0$) or total mass of recharge ($\overline{M}_r^0$) of 3 indicates that the country rock or recharge mass involved in the simulation is three times that of the magma body 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).

[13] The Linear and Non-Linear Crystallization and Melting page ("Melting Functions" button) allows a choice of melting/crystallization productivity functions, which prescribe the relationship between temperature and mass fraction of melt for each sub-system. Although linear productivity functions can be used, we recommend that the user choose nonlinear parameters because they more accurately reflect how rocks melt or magmas crystallize. The mathematical form of the nonlinear parameterization is logistical, and treatment of this function is given by *Spera and Bohrson* [2002]. To implement nonlinear logistical productivity functions, two parameters, "a" and "b", are required for pristine magma, country rock 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 1000, 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

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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 magma	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

parameters "a" and "b" are adjusted to capture the melting curves. Iterative changes in parameters "a" and "b" allow the user to define a separate productivity function for each sub-system that most closely fits the known or estimated relationship between fraction of melt and temperature. A graphical display of fraction of melt vs. temperature is provided in the code. In order to examine this plot, click the "View Non Linear Melt Chart" button. Examination of the productivity function curves is essential because values chosen for "a" and "b" must yield results that are close to 1 and 0 at the liquidus and solidus, respectively. That is, at the liquidus, almost 100% melting must occur, and at the solidus, almost 0% melting should occur. Additional treatment of this topic is deferred to section 4.

[14] 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 magma (melt + enclaves) involved in the simulation is half of the mass of the magma body (sub-system 1) 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 in the magma body, T_m, at the moment recharge magma is added to the magma body is set in Part 2 of the calculation.

[15] The X page ("X" button) allows the user to set X, the fraction of anatectic melt that enters the magma body, relative to the amount generated. X = 0 indicates that no anatectic melt enters the

magma body, whereas X = 1 means that all anatectic melt enters the magma body. In cases where X < 1, it is important to note that energy conservation requires that the appropriate mass of anatectic melt be generated, 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.

[16] 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.

[17] The "Run Equilibration" button yields n ordered pairs of T_{eq} (equilibration temperature)-$\overline{M}_a^0$ (total nondimensional 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. Table 2 describes the parameters listed in this worksheet.

3.4. Part 2 Path-Dependent Calculation: Input and Output

[18] To execute the path-dependent calculations, the user is required to choose one ordered pair (equilibration temperature (T_{eq}) - total mass of

Table 2. Explanation of Output for Part 1, Integral Energy Balance Calculation: Equilibration Parameters for EC-RAXFC Simulation[a]

Label in Code	Symbol in Text and Definition	Explanation
Norm Teq	$\overline{T}_{eq} \equiv \frac{T_{eq}}{T_{l,m}}$	nondimensional equilibration temperature of system; $T_{l,m}$ is liquidus temperature of magma body
Teq deg C	T_{eq}	equilibration temperature of system, °C
Mm	$\overline{M}_m \equiv \frac{M_m}{M_o}$	nondimensional mass of melt in magma body; M_o is initial mass of magma body (i.e., before simulation begins)
Mao	$\overline{M}_a^0 \equiv \frac{M_a^o}{M_o}$	nondimensional mass of country rock
Ma*	$\overline{M}_a^* \equiv \frac{M_a^*}{M_0}$	nondimensional mass of anatectic melt
Intermediate	—	These cells are used in subsequent calculations and should be ignored
Ms	$\overline{M}_s \equiv \frac{M_s}{M_o}$	nondimensional mass of all solids (cumulate + enclave)
fa	$f_a(\overline{T}_a)$	melt-temperature relationship for country rock (country rock melt productivity function)
fm	$f_m(\overline{T}_m)$	crystallization-temperature relationship for pristine magma (magma crystallization productivity function)
fr	$f_r(\overline{T}_r)$	crystallization-temperature relationship for recharge magma (recharge magma crystallization productivity function)

[a] Note that the abbreviations in column 1 are those in the "Equilibration" sheet presented in the code. Symbols and definitions in column 2 reflect those used in text. Note overbar denotes nondimensional parameter.

country rock sub-system ($\overline{M}_a^0$)) from the available menu. The user is then required to enter path-dependent parameters, of which there are 5 categories: Isotopes, Trace Elements, Oxygen Isotopes, Recharge, and Initial Conditions.

[19] Up to three trace element/isotope systems can be entered ("Isotopes" button). Required information includes for example, in pristine magma, element name, concentration in magma body at the start of the simulation, bulk partition coefficient (D_m^0), and enthalpy. Similar input is required for country rock and recharge magma. The enthalpy is a measure of the temperature dependence of the partition coefficient. A nonzero enthalpy permits the bulk partition coefficient to change as a function of temperature. 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 partition coefficients over a range of temperatures. By iterating, the user can identify a reasonable range of bulk partition coefficients for a single simulation. (Knowledge of the specific phases involved in a crystallizing assemblage would allow the user to identify a range of bulk partition coefficients, which can then be parameterized.) The user is also required to enter the isotope system

name (e.g., ^{87}Sr/^{86}Sr) and the isotope ratios of pristine magma (sub-system 1), 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.

[20] The user has the choice of including oxygen isotopes in the calculation ("Oxygen Isotopes" button). The ^{18}O/^{16}O for pristine magma (sub-system 1), 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.

[21] 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 body temperature. Two broad choices are provided: linear, which is considered to be a proxy for continuous recharge, and episodic. If episodic is chosen, then the user can choose to divide the total nondimensional mass of recharge magma into 1 to 20 pulses (i). For i pulses, $\Delta\overline{M}_{r,i}$ is the mass increment of recharge for pulse 1, 2, to i. $m_{r,i}$ and d_i are mathematical parameters that define the steepness and inflection of the mass of recharge-magma body temperature curve. Depending on these parameters, for each

increment of recharge mass added to the magma body, addition will occur over a small range of temperature. $T_{m,i}$ degC is the temperature in °C of the midpoint of this temperature range. To view the shape of the mass of recharge-magma body temperature curve, click the "View Recharge Event" button. Information about thermal parameters is echoed on the recharge parameters page to help the user recall thermal parameters that are relevant to setting recharge parameters. The sum of $\Delta \overline{M}_{r,i}$ (all episodes) tracks the total $\Delta \overline{M}_{r,i}$ entered by the user for all pulses and must equal $\overline{M}_r^0$.

[22] When defining the relationship between the mass of recharge magma entering the magma body and magma body 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 $\Delta \overline{M}_{r,i}$ at a $T_{m,i}$ that is close to T_{eq}. Careful examination of the recharge mass-magma body temperature curve using the "View Recharge Event" button will allow the user to identify such cases.

[23] The initial conditions page ("Initial Conditions" button) requires three actions. The first is the choice of deltaT, which is the nondimensional magma body 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 (e.g., use of very small bulk partition coefficient) or for a detailed understanding of the chemical evolution of a magmatic system. A test regarding acceptable deltaT is to run at one deltaT and then drop the deltaT again by a factor of $5-10$ and re-run the simulation. Solutions for the two simulations should be essentially identical. Additional details about deltaT are provided in section 4. 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.

[24] 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. Table 3 provides an explanation of the melt output parameters.

[25] 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.

[26] 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 to 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 are also provided. Radiogenic isotope values of cumulates are not reported because they are identical to those of melt in the magma body at each temperature step, and enclave radiogenic isotopic ratios are always those of the recharge magma. Anatectic melt isotope ratios, prior to melt incorporation into the magma body, are identical to those of the country rock; the code does not account for possible variations in anatectic melt radiogenic isotope composition due to processes such as disequilibrium melting. Oxygen isotope ratios for cumulates, enclaves, and anatectic melt are not reported because the code does not address isotopic fractionation between minerals and melt. Parameters reported in the Solids output sheet are listed in Table 4.

3.5. Graphing Capabilities

[27] 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

[28] Below, we briefly discuss three topics that will aid in using the program effectively: recognizing when numerical problems arise, use of the logistical function for nonlinear melt productivity functions, and code-imposed limitations on the degree of country rock melting.

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

Label in Code	Symbol in Text and Definition	Explanation
Norm T magma	$\overline{T}_m \equiv \dfrac{T_m}{T_{l,m}}$	nondimensional magma body temperature
T magma (deg C)	T_m	magma body temperature, degrees C[a]
Norm T assim	$\overline{T}_a \equiv \dfrac{T_a}{T_{l,m}}$	nondimensional country rock temperature
T assim (deg C)	T_a	country rock temperature, degrees C[b]
Mm	$\overline{M}_m \equiv \dfrac{M_m}{M_o}$	nondimensional mass of melt in magma body
fa	$f_a\left(\overline{T}_a\right)$	melt productivity function for country rock evaluated at T_a
Ma*	$\overline{M}_a* \equiv \dfrac{M_a*}{M_o}$	nondimensional mass of anatectic melt generated between $T_a^{\,o}$ and T_a
XMa*	$X\overline{M}_a* \equiv \dfrac{XM_a*}{M_o}$	nondimensional mass of anatectic melt added to magma body between $T_a^{\,o}$ and T_a
fm	$f_m\left(\overline{T}_m\right)$	melt productivity function for pristine magma evaluated at T_m
Mc	$\overline{M}_c \equiv \dfrac{M_c}{M_0}$	nondimensional mass of cumulates formed between $T_m^{\,o}$, $T_r^{\,o}$ and T_m (includes contribution that recharge magma makes to mass of cumulates)
Men	$\overline{M}_e \equiv \dfrac{M_e}{M_0}$	nondimensional mass of enclaves formed between $T_m^{\,o}$, $T_r^{\,o}$ and T_m
Ms	$\overline{M}_s \equiv \dfrac{M_s}{M_0}$	nondimensional mass of cumulates and enclaves (total solids) formed between $T_m^{\,o}$, $T_r^{\,o}$ and T_m
fr	$f_r\left(\overline{T}_r\right)$	melt productivity function for recharge magma evaluated at T_m
Mr	$\overline{M}_r \equiv \dfrac{M_r}{M_0}$	nondimensional mass of recharge magma added between start of simulation and T_m
Sr[c]	Sr (ppm)	elemental concentration of Sr at this T_m step
87Sr/86Sr[c]	$^{87}Sr/^{86}Sr$	isotope value at this T_m step

[a] T magma is local temperature of magma body on the path to thermal equilibration.
[b] T assim is the local temperature of country rock on the path to thermal equilibration.
[c] Output for trace elements and isotopes will vary, depending on input. If enthalpy values are nonzero, value of bulk partition coefficient is also output.

4.1. Potential Numerical Problems

[29] Because the path-dependent calculations rely on numerical solution of the coupled nonlinear equations representing conservation of energy, mass and species, numerical problems can arise during execution of Part 2 of the code. One cause of numerical problems is the use of coarse deltaT steps (chosen on the Initial Conditions page of Part 2). Numerical errors are greater in cases where $\overline{M}_a^*$ and/or $\overline{M}_r^{\,o}$ is large and/or bulk partition coefficients are extreme. Actual values of these parameters that lead to numerical problems vary, depending on a number of factors. Thus, for each simulation, it is essential to apply several simple tests that will ensure the use of proper deltaT steps.

[30] 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 last line of Melt output page 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., $\overline{M}_m$, $\overline{M}_c$, $\overline{M}_{en}$); 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.

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

Abbreviation in Code	Symbol in Text and Definition	Explanation
Norm T magma	$\overline{T}_m \equiv \dfrac{T_m}{T_{l,m}}$	nondimensional magma body temperature
T magma (deg C)	T_m	magma body temperature, degrees C
Norm T assim	$\overline{T}_a \equiv \dfrac{T_a}{T_{l,m}}$	nondimensional country rock temperature
T assim (deg C)	T_a	country rock temperature, degrees C
iMen	$i\overline{M}_{en}$	incremental mass of enclaves (nondimensional)
Men	$\overline{M}_{en}$	cumulative mass of enclaves (nondimensional)
Intermediate	—	These cells are used in subsequent calculations and should be ignored
iMc	$i\overline{M}_c$	incremental mass of cumulates (nondimensional)
Mc	$\overline{M}_c$	cumulative mass of cumulates (nondimensional)
Ms	$\overline{M}_s$	cumulative mass of solids (cumulates +enclaves) (nondimensional)
iCen [element][a]	iC_{en}	instantaneous concentration of trace element in enclaves
Cav,en	$C_{av,en}$	average concentration of trace element in enclaves
Mtr,en	$\overline{M}_{tr,en}$	mass of trace element in enclaves
iCc	iC_c	instantaneous concentration of trace element in cumulates
Intermediate	—	These cells are used in subsequent calculations and should be ignored
Mtr,c	$\overline{M}_{tr,c}$	mass of trace element in cumulates (nondimensional)
Intermediate	—	These cells are used in subsequent calculations and should be ignored
Cav,c	$C_{av,c}$	average concentration of trace element in cumulates
Cav,s	$C_{av,s}$	average concentration of trace element in solids (cumulates +enclaves)
iCa	iC_a	instantaneous concentration of trace element in anatectic melt
Cav,a	$C_{av,a}$	average concentration of trace element in anatectic melt
Mtr,a	$\overline{M}_{tr,a}$	mass of trace element in anatectic melt (nondimensional)
% error, total mass of trace element	—	Percent error in mass balance of trace element in system[b]

[a] Element name labeled in cell above. Output will vary because for each element, relevant output will be displayed.
[b] Mass balance check is described fully in section 4.

[31] As a second test, the user is referred to the mass balance output on the Solids page. This mass balance is defined by the following equation:

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

This expression represents a mass balance for a given trace element: the total mass of trace element that is initially present plus that which is added by recharge and assimilation must be balanced by the mass of trace element in the melt plus that locked up in enclaves and cumulates. If we let the left-hand side of (1) be A and the right-hand side be B, then we can compute a parameter $(\frac{A-B}{A})100$. This is the percent error of this mass balance and is precisely the number reported in the Solids output sheet (% error, total mass of trace element). 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.

[32] 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 deltaT step may be 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.

4.2. Use of Logistical Function to Define Country Rock Melt Productivity

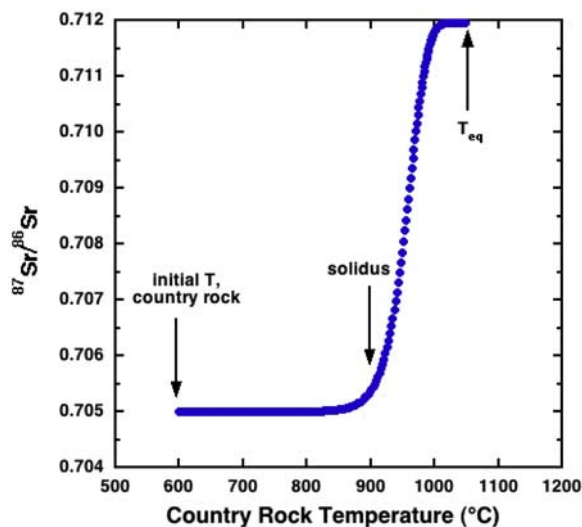[33] The mathematical form of the logistical function can yield small amounts of melting in country

Figure 2. Illustration of potential error in ^{87}Sr/^{86}Sr for case where small masses of anatectic melt are added to the magma body at temperatures below solidus. Relevant parameters: country rock "a" and "b" are 400 and −11, respectively, ^{87}Sr/^{86}Sr, Sr (ppm), and bulk partition coefficient of pristine magma and country rock are 0.705, 700, 1.5 and 0.720, 230, 0.05, respectively. ^{87}Sr/^{86}Sr at solidus is ∼0.7054, 400 ppm higher than it should be. However, note that the total range of isotope values for the magma body goes up to 0.712, and thus the error incurred at the solidus is small relative to the total isotope range manifested in the magma body. Different values of "a" and "b" can decrease this error. See text for further discussion.

rock below the solidus. Thus small masses of anatectic melt will be added to the magma body (sub-system 1) even when the country rock has not reached the solidus. For most scenarios, addition of the associated tiny masses of anatectic melt will only introduce small errors in the composition of the magma body. For example, a radiogenic isotope ratio such as ^{87}Sr/^{86}Sr might show variations of 1 to 20 ppm, compared to the value that the magma body should have when country rock reaches the solidus and the first increment of anatectic melt is added to the magma body. Such variations are within typical analytical uncertainty and therefore do not limit use of the model results. However, in cases where the bulk partition coefficient of an element in the country rock is very small (e.g., 0.05) and the radiogenic isotope ratio of country rock and pristine magma are very different (e.g., 0.720, 0.705, respectively), errors larger than typical analytical uncertainty can arise because small degree fractional melts will have very high concentrations of the element in the first

increments of melt. For particular combinations of parameters, errors of 400 ppm are possible. While such an error is typically well outside of analytical uncertainty, it is worth noting that the error introduced by this approach is small compared to the total isotope range that results in the simulation. An example below (Figure 2) elucidates this.

[34] One approach that can minimize this issue involves adjusting the country rock logistical function parameters "a" and "b" such that near the solidus, the fraction of country rock melting is very small (e.g., 0.002). Typical values that may achieve these small melt fractions are 1000 and −12, respectively. However, the user needs to carefully iterate on these values to ensure the best choice given the array of possible values for liquidus and solidus.

4.3. Limitations on Degree of Country Rock Melting

[35] There are limitations in the code that preclude the user from choosing T_{eq}, $\overline{M}_a^o$ pairs that are associated with 100% melting of country rock. This limitation is apparent in the drop down menu of pairs that the user can choose for the Part 2 calculation; only pairs that are associated with less than 100% country rock melting are possible. The code invokes this limitation to avoid a scenario where the user would choose to melt 100% of the country rock. Although this is the limitation that is hard-wired into the code, choice of T_{eq}, $\overline{M}_a^o$ pairs that are associated with relatively large degrees of melting (e.g.,<100 to ∼95%) also require caution. This is because in the Part 2 calculation, even for relatively small deltaT, the mass of country rock added in each temperature step is relatively large. This results in relatively large differences between the T_{eq} of the magma body and the T_{eq} of the country rock (e.g., >5°C) in the final temperature step of the simulation. Such large differences need to be evaluated with caution, as noted above in section 4.1.

Acknowledgments

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