Documentation for 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

Wendy A. Bohrson[1] and Frank J. Spera[2]

[1]Department of Geological Sciences, Central Washington University, Ellensburg, WA. 98926, USA, tele 509.963.2835, bohrson@geology.cwu.edu

[2]Department of Earth Science and Institute for Crustal Studies, University of California, Santa Barbara, CA. 93106, USA, 805.893.4880, spera@geol.ucsb.edu

1. Introduction

Bohrson and Spera (submitted) provides instructions for code implementation, description of input and output parameters, and estimates of typical values for some input parameters. A brief discussion elucidates measures by which the user may evaluate the quality of the output.

EC theory can be found in Spera and Bohrson (2001, 2002, 2004) and sensitivity tests and application to natural systems can be found in Bohrson and Spera (2001, 2003) and Fowler et al. (2004).

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
http://earthref.org/GERM/index.html?main.htm

To run this program, the user will need Excel 98 or higher. The code is compatible with both Mac and PC platforms.

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 access some basic information about the code.

2. 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. Below are brief descriptions of parameters and other information that may be helpful as you run EC-RAXFC.

Mass parameters in the code are all 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).

Table 1 describes thermal input parameters **(Thermal button)**, and provides typical ranges of values of basaltic to silicic composition magmas. To return to the Main Page, click the **Home button**. To move forward, click **Next**; to move back one sheet, click **Back**.

Table 1: Explanation of Thermal Input Parameters for 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	300000-450000	J/kg
hr	heat of crystallization, recharge magma	350000-500000	J/kg

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. 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**. To return the melting functions page, click the Main Menu tab.

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 can not modify these.

Click the **Home button**, which takes you to the Main Menu page.

Click **Run Equilibration button**; when the simulation is complete, a dialogue box appears EC-RAFC Equilibration complete. xx rows written to Equilibration.

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.

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

To return to the Main Menu Page, click Main Menu tab at bottom of Excel file.

3. Part 2 Path—Dependent Calculation: Input and Output

To execute the path-dependent calculations, the user is required to choose one ordered pair (equilibration temperature (T_{eq})- total mass of wall rock sub-system (M_a^o)) 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.

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 can be involved in the calculation **(Trace Elements button)**, 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 mr,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 Mr,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**. To return the Recharge Parameters page, click the Main Menu tab at the bottom of the Excel file. Information about thermal parameters is echoed on the page to help the user recall thermal parameters that are relevant to setting recharge parameters.

Example parameters for a three-pulse recharge event are listed below.

i	**$\Delta M_{r,i}$**	**$T_{m,i}$**	**$m_{r,i}$**	**$d_{,i}$**
		deg C		
1	0.1	1170	0.2	2
2	0.1	1140	0.2	2
3	0.1	1100	0.2	2

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 requires three actions **(Initial Conditions button)**. 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 may be required under certain conditions and/or for a detailed understanding of the chemical evolution of a magmatic system. 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.

Click "home" which takes you to the Main Menu page.

Run Path Dependent button yields two pages of numerical output and an additional page of associated graphs, if the graphing function is active.

A dialogue box will appear when the calculation is complete. Simulation complete. Xx rows written to Filename_xx. Click OK. The results sheet will be visible. Note that a new sheet is created for each new simulation the user completes.

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.

4. Notes about Numerical Output

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 equations:

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

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 one 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 Ma*, Mro and/or extreme bulk distribution coefficient values may require finer delta T steps.

5. Additional information

If you want to abort the simulation, hit your escape key. This will activate a box with some choices. Choose end.

If you change parameters for Part 1, you must rerun "Run Equilibration" on the Main Menu page before running Part 2. There is a dialogue box that reminds you to do this.

If you want to get rid of one or more of your results sheets, click on that sheet, and click the dialogue box that says "Discard all sheets...," located near the top of the worksheet.

6. Questions and Problems

If you have trouble downloading the program or encounter problems executing it or interpreting results, please email ecrafc@geology.cwu.edu.

7. References

Bohrson, W. A., and Spera, F. J., Energy-Constrained Open-System Magmatic Processes II: Application of Energy-Constrained Assimilation-Fractional Crystallization (EC-AFC) Model to Magmatic Systems, *Journal of Petrology*, 42, 1019-1041, 2001.

Bohrson, W. A., and Spera, F. J., Energy-constrained open-system magmatic processes IV: Geochemical, thermal and mass consequences of energy-constrained recharge, assimilation and fractional crystallization (EC-RAFC), *Geochemistry, Geophysics, Geosystems*, 4(2), 8002, doi: 10.1029/2002GC000316, 2003.

Fowler S. J., Bohrson W. A., and Spera F. J., Magmatic Evolution of the Skye Igneous Center, Western Scotland, Special Issue, *Journal of Petrology* 45: 2481-2505, 2004.

Ghiorso, M. S., and Sack, R. O., Chemical mass transfer in magmatic processes; IV, A revised and internally consistent thermodynamic model for the interpolation and extrapolation of liquid-solid equilibria in magmatic systems at elevated temperatures and pressures. *Contributions to Mineralogy and Petrology* 119, 197-212, 1995.

Spera F. J. and Bohrson W. A., Open-System Magma Chamber Evolution: an Energy-Constrained Geochemical Model Incorporating the Effects of Concurrent Eruption, Recharge, Variable Assimilation and Fractional Crystallization (EC-E'RAχFC), *Journal of Petrology* 45:2459-2480, 2004.

Spera, F. J. and Bohrson, W. A., Energy-constrained open-system magmatic processes III: Energy-Constrained Recharge, Assimilation, and Fractional Crystallization, *Geochemistry, Geophysics, and Geosystems,* (G3) 3: doi:10.1029/2002GC00315, 2002.

Spera, F. J. and Bohrson, W. A., Energy-constrained open-system magmatic processes I: general model and energy-constrained assimilation and fractional crystallization (EC-AFC) formulation, *Journal of Petrology*, 42, 999-1018, 2001.