



Energy-constrained open-system magmatic processes 3. Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RAFC)

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[1] Geochemical data for igneous rock suites provide conclusive evidence for the occurrence of open-system processes within thermally and compositionally evolving magma bodies. The most significant processes include magma Recharge (with possible enclave formation and magma mixing), Assimilation of anatectic melt derived from wallrock partial melting and formation of cumulates by Fractional Crystallization (RAFC). In this study, we extend the Energetically Constrained Assimilation and Fractional Crystallization (EC-AFC) model [Spera and Bohrson, 2001; Bohrson and Spera, 2001] to include the addition of compositionally and thermally distinct recharge melt during simultaneous assimilation and fractional crystallization. Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RAFC) tracks the trace element and isotopic composition of melt, cumulates and enclaves during simultaneous recharge, assimilation and fractional crystallization. EC-RAFC is formulated as a set of $3 + t + i + s$ coupled nonlinear differential equations, where the number of trace elements and radiogenic and stable isotope ratios modeled are t , i , and s , respectively. Solution of the EC-RAFC equations provides values for the average wallrock temperature (T_a), mass of melt within the magma body (M_m), mass of cumulates (M_{ct}) and enclaves (M_{en}), mass of wallrock involved in the thermal interaction (M_a^o), mass of anatectic melt assimilated (M_a^*), concentration of t trace elements and $i + s$ isotopic ratios in melt (C_m), cumulates (C_{ct}), enclaves (C_{en}), and anatectic melt (C_a) as a function of magma temperature (T_m). Input parameters include the equilibration temperature (T_{eq}), the initial temperature and composition of pristine melt (T_m^o , C_m^o , ϵ_m^o), recharge melt (T_r^o , C_r^o , ϵ_r^o), and wallrock (T_a^o , C_a^o , ϵ_a^o), temperature-dependent trace element distribution coefficients (D_m , D_r , D_a), heats of transition for wallrock (Δh_a), pristine melt (Δh_m), and recharge melt (Δh_r), and the isobaric specific heat capacity of assimilant ($C_{p,a}$), pristine melt ($C_{p,m}$), and recharge melt ($C_{p,r}$). The magma recharge mass function, $M_r(T_m)$, is specified a priori and defines how recharge magma is added to standing magma. The present EC-RAFC simulator incorporates a weak coupling to major element mass balance and phase relations based on laboratory experiments or Gibbs Energy minimization [e.g., Ghiorso, 1997]. EC-RAFC can be applied to a variety of magmatic systems including volcanic suites that show evidence of magma mixing, layered mafic intrusions, and granitoid plutons. Predictions for masses, as well as compositions of magmatic products, are part of the EC-RAFC solution. The “systems” approach provides an opportunity to quantitatively assess the roles of assimilation, fractional crystallization, and magma recharge in magma evolution using trace element and isotopic constraints together with energy conservation.

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1. Introduction

[2] Magmatism represents an important mechanism for transport of energy and material within the mantle and between the mantle and crust on Earth and other terrestrial planets. The simultaneous occurrence of magma recharge, assimilation, and fractional crystallization (RAFC) leaves a distinctive trace element and isotopic imprint on magmatic products (melts and solids). The preserved compositional record allows one to reconstruct the history of the magmatic system, which reveals much about the formation of continental and oceanic crust as well as the thermal evolution of the Earth on both global and regional scales. The essential premise of our work, indeed the sine qua non, is that the thermal evolution of a magmatic system cannot be divorced from its compositional evolution. Models that achieve energy balance or mass balance in isolation are, at best, inchoate.

[3] Although, in principle, development of a comprehensive model for open system magmatic evolution is straightforward, complications arise due to the unknown configuration of magma bodies, the lack of a general thermodynamic model incorporating all phases and components (major, minor and trace elements including isotopic ratios), incomplete information on the transport properties of magma and an incomplete understanding of the transport phenomena involved in the coupled processes of assimilation, fractional crystallization and recharge. In addition, the effects of host rock

partial melting, incomplete homogenization of melt within a magma body and the large variations in host rock environments bedevil attempts to holistically model specific systems a priori. Fortunately, the situation is not completely hopeless. The relationship between RAFC processes and the energetics of magmatic systems provides a basic constraint on partial melting, crystallization and enthalpy transfer if a suitable representation of the system can be arranged. When coupled with trace element and isotope material balance expressions (conservation of total mass and trace species), the energy constraint enables development of a self-consistent algorithm for calculation of geochemical paths. In Energy-Constrained Recharge, Assimilation, and Fractional Crystallization (EC-RAFC), the geochemical path refers to the progression of wall-rock temperatures (T_a), trace element concentrations and isotope ratios in unmixed anatectic melt, magma body melt and crystallized solids (cumulates and enclaves) as a function of the melt temperature T_m . The solid products of an RAFC event are of two types and include *cumulates* produced by fractional crystallization of standing magma as well as the solids (herein termed *enclaves*) produced by the rapid chilling of all or a portion of injected recharge melt.

[4] The purpose of this paper is to present a description of the EC-RAFC model including a detailed derivation. In a companion paper [Bohrson and Spera, 2002], the EC-RAFC model is applied to some common petrologic scenarios. The present

work builds upon the EC-AFC (Energetically Constrained Assimilation and Fractional Crystallization) model that tracks the trace element and isotopic evolution of a batch of magma undergoing concurrent assimilation and fractional crystallization [Spera and Bohrson, 2001]. EC-AFC was applied to several natural systems where geologic evidence suggested magma recharge was probably not significant [Bohrson and Spera, 2001]. The addition of recharge magma to an evolving magma body is not uncommon based on observations from many layered intrusions [Cawthorn, 1996] and ideas on the role of mafic magma underplating in the formation of continental crust and oceanic plateaus [Coffin and Eldholm, 1994]. Evidence of mixed and comingled magmas is very common in intermediate to silicic composition continental and island arc magmatic systems as well [e.g., Snyder, 1997; Snyder and Tait, 1998]. In particular, the heat needed to trigger crustal anatexis may be advected into the source region by intrusion from below of hotter, more mafic, magma [e.g., see Raia and Spera, 1997, and references therein].

[5] A historical review of RAFC and AFC modeling in geochemistry may be found in the work of Spera and Bohrson [2001] and is not repeated here. Some existing RAFC geochemical models are cited and discussed in the treatise by Albarède [1995, see especially p. 501–522]. A limitation common to previous studies is the lack of self-consistent energetics and the inability to handle the effects of wallrock partial melting or the consequences of addition of recharge magma of arbitrary composition and specific enthalpy. Although a few extant models do consider some of these features, no model does so comprehensively and self-consistently.

[6] The EC-RAFC model is not a dynamical or transport model. Although this may seem debilitating, it is precisely because EC-RAFC considers only the energetics and material balances that it may be applied to a variety of systems in the presence of incomplete information, the usual situation in petrochemical modeling efforts. What is lost in terms of absolute timescale [Hawkesworth *et al.*, 2000; Edwards and Russell, 1998; Russell and Hauksdottir, 2001] is gained in terms of generality. In order to make a full accounting of the magma dynamics for

specific magmatic systems a great deal of information, usually unavailable, must be known. For example, in order to quantify magma convection, magma mixing, the nucleation, growth and separation (gravitational and otherwise) of crystals and rates of assimilation and solidification, the size, shape and surface area of the magma body as well as the detailed characteristics of the environment (among a host of additional factors) must be known. All of this information is rarely available. Furthermore, during protracted evolution of a magmatic system these factors vary temporally in ways that are difficult to predict. Although one can make assumptions and build forward models (see Spera *et al.* [1995], Jaupart and Tait [1995], Campbell [1996], Tait and Jaupart [1996], Barboza and Bergantz [1998], and Snyder and Tait [1998] for a few illustrative examples), these models can rarely be applied to particular magmatic systems for which a large amount of geochemical data may exist. The goal of the EC-RAFC approach is to be able to assemble a reasonable first-order physical model with available geochemical data to extract petrological insight from specific magmatic systems.

2. Composite EC-RAFC Model: Systems Approach

[7] In EC-RAFC, a magmatic system is modeled as a composite system adiabatically sealed from its surroundings, as depicted in Figure 1. The subsystems that make up the composite system include wallrock, a standing (initially pristine) magma body and a reservoir of recharge melt. Each of these subsystems is separated from one another by diathermal and “osmotic” boundaries that allow heat exchange and partial chemical species exchange during the RAFC event. The subsystems themselves can be viewed as composite systems so that compositionally zoned magma, recharge magma of varying composition and specific enthalpy (enthalpy per unit mass) and imperfect extraction of anatectic melts can be incorporated into the EC-RAFC scheme. The EC-RAFC version presented below applies to homogeneous (nonzoned) magma bodies replenished by recharge magma of fixed composition (but different than standing magma) and temperature. The anatectic melt extraction factor, χ , is unity, which means

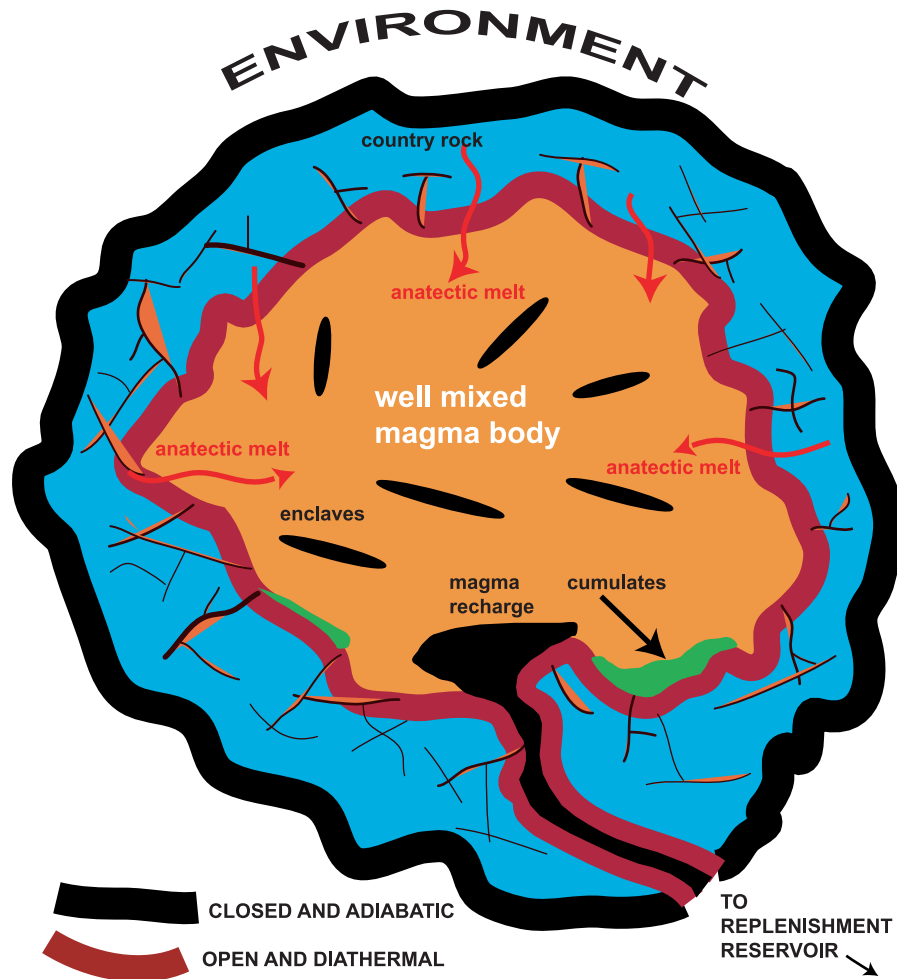


Figure 1. Thermodynamic system approach to RAFC processes. The composite magmatic system is composed of three sub-systems: a magma body (melt + cumulates + enclaves), wall rock of initial mass M_a^o and replenishment reservoir of total mass M_r^o . The subsystems are separated from the environment (surroundings) by rigid, impermeable and adiabatic boundaries during the RAFC event. At the start of the RAFC interaction, boundaries between all subsystems are made diathermal and “osmotic”, and the composite system relaxes to a state of equilibrium consistent with thermodynamic constraints. During the RAFC event, anatectic melt of mass M_a^* is added to and homogenized with melt in the standing magma body. Cumulates (M_{c_i}) form by fractional crystallization and are in isotopic and trace element equilibrium with coexisting melt within the magma body. The fate of incrementally added recharge melt depends on the initial temperature of the recharge system (T_r^o) relative to the temperature of standing magma (T_m) at the instant of recharge intrusion. If $T_r^o > T_m$, a fraction of recharge melt, determined from the melt productivity function, $f_r(T_m)$, chills to form enclaves (see text). The composition of enclaves is governed by fractional crystallization of pristine recharge melt. That part of the recharge melt that does not chill to form enclaves is assumed to homogenize with standing magma.

that all anatectic melt generated by partial melting of wallrock is added to and homogenized with standing melt (see *Spera and Bohrsen* [2001] for a discussion). Because no anatectic melt remains in the country rock, this version of EC-RAFC provides a maximum limit for magma contamination consistent with the energetics.

[8] A thermodynamic description of a magmatic system and its surroundings during an RAFC event

serves to outline the salient features of the EC-RAFC model and illustrates the progression of states along the EC-RAFC geochemical path (Figure 2). Nomenclature used in this discussion and in the differential equations that follow is defined in Table 1. The initial state (Figure 2a) is a composite magmatic system composed of three subsystems: country rock of mass M_a^o at mean initial temperature T_a^o , a pristine batch of chemically homogeneous melt of mass M_o at initial temperature T_m^o (“standing magma”)

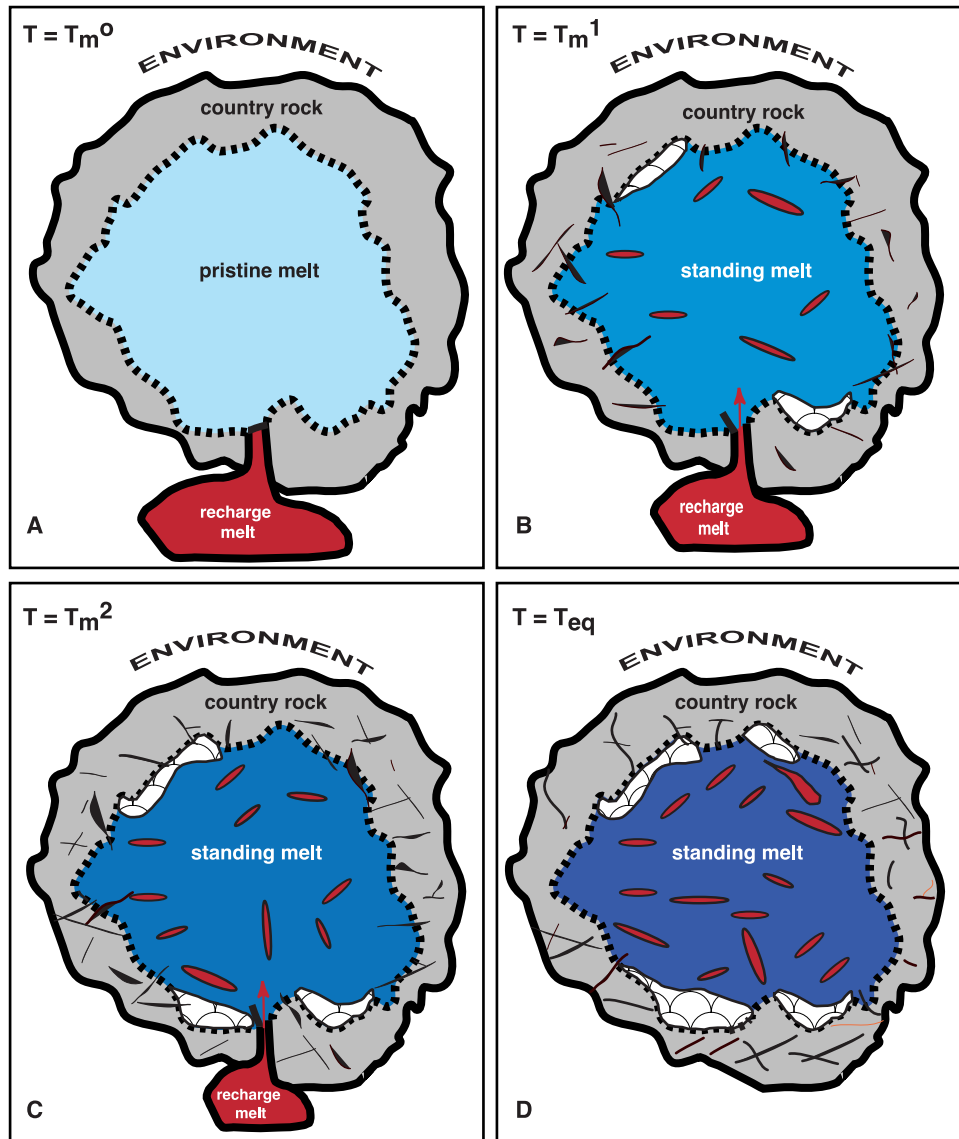


Figure 2. Depiction of an RAFC event for magmatic composite system. (a) Initial state: Mass M_0 of pristine standing melt at temperature $T = T_m^0$ and composition $C_m^0, \epsilon_m^0, \delta_m^0$ separated from country rock of composition $C_a^0, \epsilon_a^0, \delta_a^0$ at average temperature T_a^0 by a diathermal, rigid boundary. The melt body is connected to a reservoir of recharge melt of distinct temperature T_r^0 and composition ($C_r^0, \epsilon_a^0, \delta_a^0$), (b) Intermediate state (early part of RAFC event): Melt has cooled from T_m^0 to T_m^1 and country rock restite is heated from T_a^0 to T_{a1} . Cumulates (bubble foam) have formed by fractional crystallization. Standing melt is contaminated by assimilation of anatectic liquids (black dikes). Some recharge melt has been chilled to form enclaves (red disks), (c) Intermediate state (later part of RAFC event): Melt cooled to T_m^2 and wallrock heated to T_{a2} . Masses of cumulates and enclaves have increased compared to earlier state, (d) Final state: Thermal equilibrium is attained within the composite system ($T_a = T_m = T_{eq}$) that remains isolated from its surroundings. All recharge (M_r) has been added and the magma body consists of melt, cumulates and enclaves.

and a compositionally distinct (but homogeneous) recharge melt reservoir of mass M_r^0 and initial temperature T_r^0 . The trace element and isotopic compositions of all materials are specified. Once the RAFC process is initiated (Figure 2b), the country rock-magma body boundary is diathermal and open, allowing exchange of

enthalpy and addition of anatectic melt generated by partial melting in the country rock to the standing magma. Recharge melt is added during the RAFC event according to an ab initio (user-defined) prescription $M_r = M_r(T_m)$, where T_m is the temperature of standing melt. T_m varies from T_m^0 to the (final) equilibration temperature, T_{eq} , set by the

Table 1. Nomenclature

Symbol	Definition	Unit
T_m^o	initial standing melt temperature	K
T_r^o	initial recharge melt temperature	K
$T_{1,m}$	pristine standing melt liquidus temperature	K
T_{eq}	equilibration temperature	K
T_m	standing melt temperature	K
T_a	temperature of country rock	K
$T_{1,a}$	wall rock liquidus temperature	K
T_a^o	initial wallrock temperature	K
$T_{1,r}$	recharge melt liquidus temperature	K
$T_{r,i}$	Temperature midpoint of i th recharge interval	K
Δh_a	enthalpy of fusion of assimilant	J/kg
Δh_m	enthalpy of crystallization of standing magma	J/kg
Δh_r	enthalpy of crystallization of recharge magma	J/kg
$C_{p,m}$	magma isobaric specific heat capacity	J/kg K
$C_{p,a}$	assimilant isobaric specific heat capacity	J/kg K
$C_{p,r}$	recharge melt specific heat capacity	J/kg K
$M_r(T_m)$	mass of recharge magma	kg
M_r^o	mass of recharge magma added during RAFC event	kg
M_o	mass of initial magma	kg
M_{ct}	mass of cumulates	kg
M_{en}	mass of enclaves	kg
M_s	total mass of solids (cumulates plus enclaves)	kg
$\Delta M_{r,i}$	i th increment of recharge mass addition	kg
N_r	number of episodes of recharge addition	
m_i	parameter in recharge addition mass function	K^{-1}
d_i	parameter in recharge addition mass function	
h_{lib}	total heat liberated by magma	J
h_{abs}	total heat absorbed by country rock	J
Δh_a	specific fusion enthalpy of wallrock	J/kg
Δh_m	specific crystallization enthalpy of standing magma	J/kg
Δh_r	specific crystallization enthalpy of recharge melt	J/kg
M_m	mass of melt in magma body	kg
M_a^*	mass of anatectic melt	kg
M_a^o	mass of country rock involved in RAFC event	kg
ΔH_a	enthalpy of wallrock/anatectic melt partition coefficient	J/mol
ΔH_m	enthalpy of cumulate/standing melt partition coefficient	J/mol
ΔH_r	enthalpy of enclave/recharge melt partition coefficient	J/mol
χ	melt extraction efficiency	
C_a	concentration of trace element in country rock ^a	ppm
C_r	concentration of trace element in recharge melt	ppm
C_m	concentration of trace element in standing melt	ppm
C_{en}	concentration of trace element in enclave	ppm
\hat{C}_a	average concentration of anatectic melt along path $T_a^o \rightarrow T_m$	ppm
\hat{C}_{ct}	Instantaneous concentration of trace element in cumulate	ppm
\hat{C}_{ct}	average concentration of cumulates along path $T_m^o \rightarrow T_m$	ppm
\hat{C}_{en}	average concentration of enclaves along path $T_m^o \rightarrow T_m$	ppm
D_m	bulk distribution coefficient between cumulate and melt	
D_a	bulk distribution coefficient between wallrock and anatectic melt	
D_r	bulk distribution coefficient between enclave and recharge melt	
$s \equiv \frac{C_r}{C_a}$	ratio of initial concentration of trace element in country rock and pristine magma	
$t \equiv \frac{C_r}{C_m}$	ratio of initial concentration of trace element in recharge melt and pristine magma	
ϵ_m	isotopic ratio in standing melt	
ϵ_r	isotopic ratio in recharge melt	
ϵ_a	isotopic ratio in assimilant	
δ_a	oxygen isotopic composition of assimilant	
δ_m	oxygen isotopic composition of standing magma	
δ_r	oxygen isotopic composition of recharge melt	
$f_m(T)$	melt productivity of pristine initial standing melt composition	
$f_a(T)$	melt productivity of wallrock composition	
$f_r(T)$	melt productivity of recharge melt composition	

Table 1. (continued)

Symbol	Definition	Unit
$\bar{M}_{en} \equiv \frac{M_{en}}{M_o}$	non dimensional mass of enclaves	
$\bar{M}_{ct} \equiv \frac{M_{ct}}{M_o}$	nondimensional mass of cumulates	
$\bar{M}_s \equiv \frac{M_s}{M_o}$	nondimensional mass of all solids (cumulates plus enclaves)	
$\bar{M}^a \equiv \frac{M^a}{M_o}$	nondimensional mass of assimilant	
$\bar{T}_{eq} \equiv \frac{T_{eq}}{T_{lm}}$	nondimensional equilibration temperature	
$\bar{T}_a \equiv \frac{T_a}{T_{lm}}$	nondimensional assimilant temperature	
$\bar{T}_m \equiv \frac{T_m}{T_{lm}}$	nondimensional magma temperature	
$\bar{M}_m \equiv \frac{M_{lp}}{M_o}$	nondimensional melt fraction in magma body	
$\bar{C}_a \equiv \frac{C_a}{C_o}$	nondimensional concentration of trace element in anatectic melt	
$\bar{C}_r \equiv \frac{C_r}{C_o}$	nondimensional concentration of trace element in recharge magma	
$\bar{C}_m \equiv \frac{C_m}{C_o}$	nondimensional concentration of trace element in melt	

^a In text and equations, initial values of trace element concentrations and isotopic ratios denoted by superscript ^o, e.g., C_a^o is the initial concentration of trace element in wallrock.

modeler [see *Spera and Bohrsen, 2001*]. T_m (i.e., temperature *not* time) is used as the variable to monitor the progress of the RAFC event in the differential equations defining the geochemical path. Although time is not considered in the thermodynamic model, T_m serves as time's arrow [Eddington, 1930; De Donder and Van Rysselberghe, 1967; Prigogine, 1967]. Like time, T_m monotonically decreases from the initial value to the final, user-defined equilibration temperature.

[9] The thermal consequences of recharge depend on the initial temperature of recharge melt, the recharge melt productivity function, $f_r(T)$, and the temperature of standing magma at the time of recharge. In the current version of EC-RAFC, the initial temperature of recharge melt is set equal to the liquidus temperature of recharge magma, $T_{l,r}$. If $T_r^o < T_m$, heat is exchanged between standing magma and recharge magma until recharge magma attains T_m . Addition of recharge melt under these conditions results in a “wave” of cumulate formation. The mass of cumulates produced depends upon the partitioning of sensible and latent heat *via* the melt productivity function for pristine magma, $f_m(T)$. In contrast, if $T_r^o > T_m$, the fraction $1 - f_r(T_m)$ of recharge mass solidifies by closed system fractional crystallization upon intrusion into cooler standing magma. The solid (chilled) product of this thermal interaction is defined as an *enclave* [Didier and Barbain, 1991; Furman and Spera, 1985] in the EC-RAFC formulation.

[10] Because the term *enclave* has been defined in various ways, a brief review of its definition and its

precise meaning in the EC-RAFC context is given here. *Best and Christiansen* [2001] state that a *mafic inclusion* or *enclave* can originate in a number of ways. These include (briefly): (1) *xenolith*: undigested foreign country rock (wallrock), (2) *restite*: fragment of residual source rock remaining after melt extraction, subsequently entrained by ascending magma, (3) *autolith*: partially to wholly solidified part of an intrusion that mixes (as a “brittle” fragment) with surrounding (essentially identical) magma, and (4) *viscous blob*: intrusion of magma of distinct viscosity (composition and temperature) into a second (compositionally and thermally) distinct magma. The blob may solidify, forming an aphanitic (microgranular) inclusion if homogenization by advective mixing is retarded. As noted, for example by R.A. Wiebe and coworkers [Wiebe, 1993; Wiebe and Snyder, 1993; Wiebe, 1994; Wiebe and Adams, 1997; Waight et al., 2001; Wiebe et al., 2001], the form intruded recharge magma assumes may vary from pillowed blobs to larger sheets.

[11] In EC-RAFC, an enclave corresponds most closely to definition (4) above. That is, an enclave refers to the “chilled” solid formed when recharge melt at T_r^o intrudes standing magma at T_m when $T_m < T_r^o$. The mass increment of the recharge material that solidifies is $[1 - f_r(T_m)] dM_r$ where dM_r is the differential increment of total recharge mass added. The trace element composition of the enclave is determined assuming closed system fractional crystallization of recharge magma. Enclave isotopic composition is identical to that

of recharge melt since no isotopic fractionation occurs during closed system fractional crystallization. Once an enclave forms, it does not react with melt and remains solid throughout the RAFC event. Due to enclave formation, the portion of recharge melt remaining after enclave formation is compositionally evolved compared to the initial recharge composition. This residual recharge melt homogenizes with standing melt by advective and diffusive mixing. Unlike enclaves, cumulates form in chemical equilibrium with standing melt. Hence in EC-RAFC, enclaves and cumulates must be independently tracked. In fact, the ratio of enclave to cumulate provides valuable insight into the RAFC “event” [Bohrson and Spera, 2002].

[12] Heat derived from magma cooling and cumulate formation and addition of recharge (when thermal initial conditions are appropriate) heats a finite mass of wallrock (M_a^o , see below) and induces anatexis provided the country rock solidus (T_s) is exceeded. The EC-RAFC event is completed (Figure 2d) when the temperature of the wallrock restite (that part of country rock that remains solid) is equal to T_m and both equal T_{eq} . That is, at the completion of the RAFC event, $T_a = T_m = T_{eq}$. In cases where all the country rock involved in the interaction melts, the equilibration condition is $T_m = T_{eq}$. When T_{eq} is reached, the RAFC system consists of four parts: (1) a mass M_m of homogeneous standing melt, (2) a mass M_{ct} of cumulates of variable composition, (3) a mass M_{en} of chill solids (enclaves) of variable composition formed by fractional crystallization of pristine recharge melt, and (4) a mass of wallrock restite $M_a^o - M_a^*$ with trace element composition that reflects the extraction of anatectic melt of mass M_a^* .

[13] A great deal of information that can be exploited to reconstruct the RAFC history of a magmatic system is stored in the compositional record (trace element concentrations and isotopic ratios) of the solids (cumulates and enclaves, if present). Information is also stored in the sequence of melts formed during the RAFC event. Such liquids are sometimes trapped as melt (glass) inclusions within crystalline phases. Although interpretation of these data is never trivial, the RAFC model provides a means to link

observed geochemical information from melts and solids into a consistent scheme.

[14] To uniquely define an RAFC event, an integral energy balance providing an explicit connection between the mass and thermal properties of all subsystems for a set of initial conditions and the user-defined equilibration temperature is made. The integral equation enables determination of the mass of wallrock, M_a^o , that thermally equilibrates (and possibly partially melts) with the other subsystems during the RAFC event. Once M_a^o has been determined, path-dependent parameters, such as trace element and isotope characteristics of melt and solids (cumulates and enclaves) are determined by solution of a system of first-order coupled nonlinear differential equations. The equations express conservation of energy, mass, species and isotope balance as a function of melt temperature for $T_m \in [T_m^o, T_{eq}]$. The energy constraint fundamental to the EC approach dictates that the enthalpy released by magma cooling and solids formation is absorbed by wallrock and potentially induces country rock anatexis. The extent of wallrock partial melting depends on the melt productivity of wallrock, $f_a(T_a)$, its average initial temperature (T_a^o), average isobaric specific heat capacity ($C_{p,a}$) and the enthalpy of fusion (Δh_a). There can be a positive or negative correlation between the extent of anatexis and the addition of recharge magma depending upon the initial temperature and thermodynamic properties of recharge melt relative to T_m at the time of intrusion.

3. Composite EC-RAFC Model: Computation of the Geochemical Path

[15] In the EC-RAFC model, standing melt and wallrock have unique initial trace element (C_m^o , C_a^o) and isotopic (ϵ_m^o , δ_m^o , ϵ_a^o , δ_a^o) compositions. Recharge melt, with distinct trace element (C_r^o) and isotopic (ϵ_r^o , δ_r^o) compositions at initial temperature T_r^o , is added to standing magma according to the a priori relation $M_r = f(T_m)$. The total mass added to the magma body during the RAFC event is M_r^o and is evaluated according to $M_r^o = f(T_{eq})$. A flexibility of the EC-RAFC model is that the recharge addition function can be arbitrarily specified. Wallrock partial melts are extracted, thermally

equilibrated with, and homogenized with standing melt. Tracking the geochemical path during RAFC demands an accurate rendering of phase relations which govern bulk trace element mineral/melt distribution coefficients as well as the thermal properties and melt productivity functions for pristine magma, wallrock and recharge magma. Results from both experimental phase equilibria and thermodynamic modeling [e.g., *Ghiorso*, 1997] may be used to constrain the thermodynamics of melting. These constraints are encompassed into EC-RAFC modeling *via* melt productivity functions for assimilated, magma and recharge compositions. The solution of the conservation equations provides values for the mass of heated wallrock (M_a^o), the amount of anatectic melt (M_a^*) generated, the mass of melt in the chamber (M_m), and the mass of cumulates (M_{ct}) and enclaves (M_{en}) as a function of T_m along the path $T_m^o \rightarrow T_{eq}$. In addition to masses, trace element concentrations and radiogenic and oxygen isotope ratios in melt, cumulates and enclaves at each temperature along the path $T_m^o \rightarrow T_{eq}$ are determined.

[16] In the following sections, mathematical details of the EC-RAFC algorithm, including auxiliary relations, are developed. The first section details the parameterization of the mass recharge function, $M_r(T_m)$, and the nonlinear melt productivity functions $f_a(T)$, $f_m(T)$ and $f_r(T)$. This is followed by derivation of the EC-RAFC algorithm in two parts. The first is an integral energy conservation statement that provides a set of ordered triplets (T_{eq} , M_a^o , M_r^o) for specific thermodynamic properties and initial conditions. A particular choice of T_{eq} is made by the modeler based upon geologic knowledge of the magmatic system under study (see *Spera and Bohrson* [2001] for details). Once T_{eq} has been chosen, the second part of the calculation, involving solution to the path-dependent differential equations, gives the chemical and thermal evolution of the melt, wallrock, cumulates and enclaves along the RAFC temperature trajectory $T_m^o \rightarrow T_{eq}$.

4. Mathematical Details

4.1. Magma Recharge Functions

[17] In EC-RAFC, recharge melt is added to standing magma during the approach to thermal equi-

librium. In general there are no constraints on the cumulative recharge mass addition function, $M_r(T_m)$ except that it be monotonic and positive. Two particular forms are especially useful as “end-member” models. The simplest recharge addition function is the linear one,

$$\overline{M}_r(\overline{T}_m) = \overline{M}_r^o(T_{l,m}\overline{T}_m - T_m^o)/(T_{eq} - T_m^o) \quad (1)$$

Non-dimensional quantities are denoted by overbars and defined along with other parameters in Table 1. In this case, recharge is added to the magma body as a linear function of T_m . Examination of the trace element stratigraphy of many layered intrusions suggests that a more realistic end-member mass recharge model is the multiple pulse or episodic input model. For example, in the Muskox layered intrusion, Northwest Territories, Canada, each of the 25 cyclic units in the cumulate pile has been interpreted to represent a pulse of magma recharge [*Irvine*, 1980]. The multiple pulse input of recharge is modeled as follows. At some set of predetermined small temperature intervals (the i th with midpoint $T_{r,i}$), the i th pulse of recharge magma of mass $\Delta M_{r,i}$ is added to the evolving magma body. There may be an arbitrary number (N_r) of episodes of melt input. The cumulative mass of recharge melt for multiple recharge events takes the form:

$$\overline{M}_r(\overline{T}_m) = \sum_{i=1}^{N_r} \frac{\Delta \overline{M}_{r,i}}{\{1 + \exp[m_i(T_{l,m}\overline{T}_m - T_{r,i})]\}^{d_i}} \quad (2)$$

In (2), the factors m_i and d_i control the width and slope of the recharge mass function; $T_{r,i}$ is the midpoint of the temperature interval during which the pulse of recharge melt is added and $\Delta M_{r,i}$ is the mass of the i th pulse. Because the mass input function can be made arbitrarily steep, $T_{r,i}$ is essentially the temperature of standing magma at the instant of recharge addition. In Figure 3, an example of a three-pulse input function $M_r(T_m)$ is given. The sum of the increments of recharge equals the total mass of recharge added during the RAFC event ($\sum_{i=1}^{N_r} \Delta M_{r,i} = M_r^o$). By use of (2), one may specify pulses of arbitrary mass and duration at specific narrow temperature intervals of a few degrees in the temperature interval $T_m^o \rightarrow T_{eq}$. Differentiation of (2) gives a nonlinear ordinary

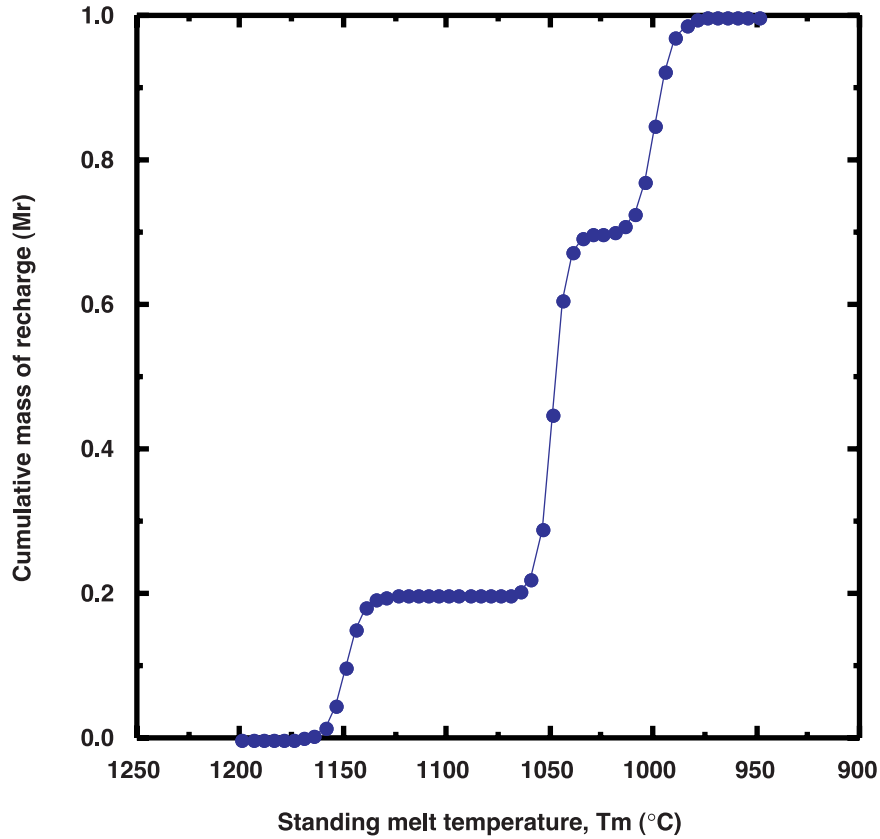


Figure 3. Example of episodic addition of recharge melt to a standing magma body. $M_r(T_m)$ is the cumulative mass of recharge material added to the magma body as a function of standing melt temperature, T_m . T_m decreases from the initial value T_m^0 to the equilibration value T_{eq} . The function $M_r(T_m)$ is defined by specifying the number of episodes (N_r) of recharge. The example shown is for a three-pulse RAFC event ($N_r = 3$). Four parameters are needed to define each pulse of recharge (see (2) in text). For the example shown, they are $\Delta M_{r,i}$, $T_{r,i}$, m_i , d_i : (0.2, 1150°C, 0.12, 2), (0.5, 1050°C, 0.15, 2), (0.3, 1000°C, 0.15, 1.5) with $T_m^0 = 1200^\circ\text{C}$ and $T_{eq} = 950^\circ\text{C}$. M_r^0 , the sum of the three pulses equals = 1.0 in the example shown.

differential equation for the variation of the mass of recharge magma with T_m :

$$\frac{d\bar{M}_r}{dT_m} = - \sum_i^{N_r} T_{l,m} d_i m_i \Delta \bar{M}_{r,i} \exp[m_i (T_{l,m} \bar{T}_m - T_{r,i})] \cdot \{1 + \exp[m_i (T_{l,m} \bar{T}_m - T_{r,i})]\}^{(-d_i+1)} \quad (3)$$

4.2. Melt Productivity Functions

[18] Melt productivity functions defined for the EC-RAFC formulation represent the relationships between mass fraction of liquid and temperature for the fixed compositions of unmodified wall-rock, pristine standing magma before RAFC and recharge melt ($f_a(T)$, $f_m(T)$ and $f_r(T)$, respectively). The required melt productivity relations

may be determined by laboratory experiment, MELTS [Ghiorso, 1997] simulation or by some other parameterization. Productivity functions must be defined in order to perform a geochemical path simulation using the EC-RAFC model.

[19] The simplest form for the melt productivity function is linear:

$$f_a(T) = \frac{T - T_s}{T_{l,a} - T_s}, f_m(T) = \frac{T - T_s}{T_{l,m} - T_s} \text{ and } f_r(T) = \frac{T - T_s}{T_{l,r} - T_s} \quad (4)$$

for assimilant, magma and recharge compositions, respectively. Linear melt production is a crude end-member behavior. An example of a model binary system that approximately follows linear melting is the system $\text{CaAl}_2\text{Si}_2\text{O}_8\text{-NaAlSi}_3\text{O}_8$ at low pressure. More realistic parameterizations for

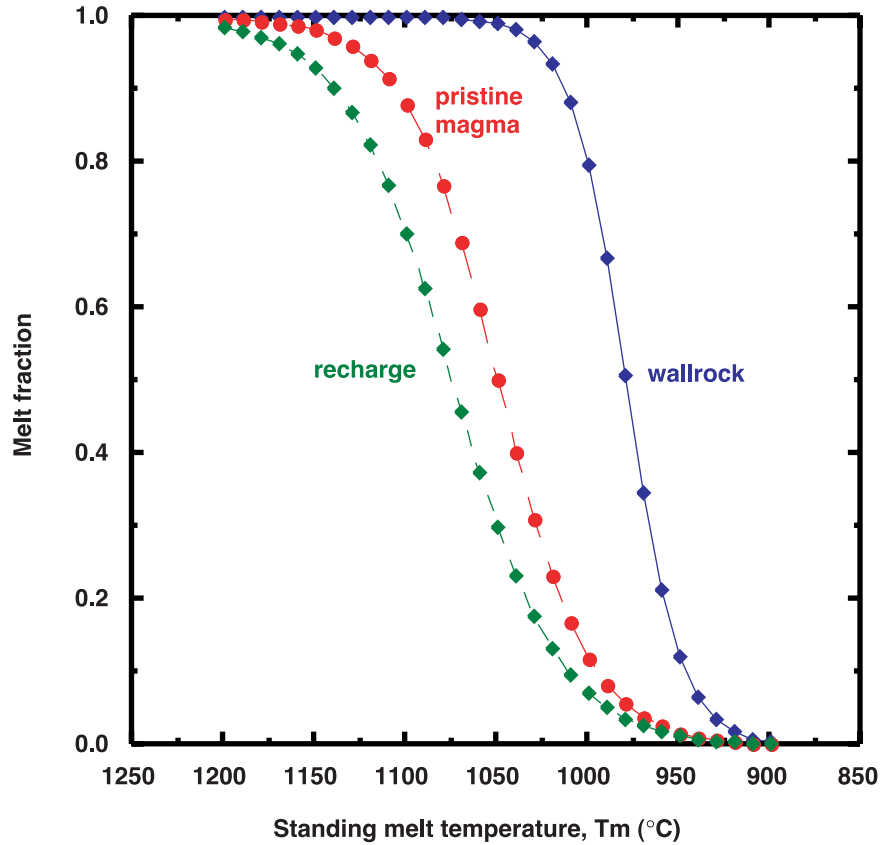


Figure 4. Illustrative melt productivity functions which give the relationship between the fraction of melt and the temperature for given (fixed) bulk compositions of wallrock (a), pristine standing melt (m) and recharge (r). The form of the melt productivity function is given by equation (7) in the text. The parameters are (a) wallrock: $T_{l,a} = 1050^{\circ}\text{C}$, $a_a = 200$, $b_a = -10$; (b) pristine melt, $T_{l,m} = 1200^{\circ}\text{C}$, $a_m = 400$, $b_m = -12$; (c) recharge, $T_{l,r} = 1250^{\circ}\text{C}$, $a_r = 400$, $b_r = -12$.

multicomponent silicate compositions are given by the logistical form:

$$f_a(\phi_a) = (1 + a_a \exp(b_a \phi_a))^{-1}, f_m(\phi_m) = (1 + a_m \exp(b_m \phi_m))^{-1} \quad (5)$$

and $f_r(\phi_r) = (1 + a_r \exp(b_r \phi_r))^{-1}$

where

$$\phi_a(T) = \frac{T_{l,m}\bar{T} - T_s}{T_{l,a} - T_s}, \phi_m(T) = \frac{T_{l,m}\bar{T} - T_s}{T_{l,m} - T_s} \quad \text{and} \quad (6)$$

$$\phi_r(T) = \frac{T_{l,m}\bar{T} - T_s}{T_{l,r} - T_s}$$

The melt productivity functions based on (5) and (6) reduce to:

$$f_j(\phi_j) = \left\{ 1 + a_j \exp \left[b_j \left(\frac{\bar{T} - \bar{T}_s}{\bar{T}_{l,j} - \bar{T}_s} \right) \right] \right\}^{-1} \quad (7)$$

Some illustrative melt productivity curves based on (7) are shown in Figure 4. The parameters a_j and b_j with $j \in \{a, m, r\}$ are empirically determined by fit of experimental or MELTS [Ghiorso, 1997] data to equation (7). The parameters \bar{T}_s and $\bar{T}_{l,j}$ represent dimensionless solidi and liquidi of composition j where $j \in \{a, m, r\}$. An even more general melt productivity relation based upon a four-parameter logistic curve enables one to consider multiply stepped melt production relations common in systems with complex phase relations. This relation takes on the form:

$$f_j(\bar{T}) = \sum_{i=1}^{\zeta} \frac{\alpha_i}{\{1 + \exp[\beta_i(\bar{T} - \Omega_i)]\}^{\lambda_i}} \quad (8)$$

where ζ is the number of steps needed to accommodate multiply stepped melt productivity

curves and the α_i , β_i , Ω_i , and λ_i are fit parameters based on laboratory experiments or MELTS calculation. In practice, the form (7) works quite well and, with judicious choice of a_j and b_j , faithfully captures the sigmoidal form of melt productivity functions for common compositions.

4.3. Integral Energy Balance

[20] The integral enthalpy balance provides a constraint on the geochemical path followed by melt, cumulates, and enclaves during EC-RAFC. The balance defines an algebraic relation among three quantities: the mass of country rock involved in the RAFC event, M_a^o , the total mass of added recharge, $M_r^o \equiv M_r(T_{eq})$, and the equilibration temperature, T_{eq} . Not all wallrock necessarily melts, although all of it does eventually come to thermal equilibrium with melt, cumulates and enclaves. The energy conservation statement incorporates heating and partial melting of country rock, magma cooling and cumulate formation, addition of recharge melt, and possible enclave formation. The parameters required for the integral balance include the melt productivity functions for country rock, standing and recharge magmas (f_a , f_m and f_r , respectively), enthalpy of crystallization for standing and recharge magmas (Δh_m and Δh_r), the fusion enthalpy of wallrock (Δh_a) and the average isobaric specific heat capacity of all compositions ($C_{p,a}$, $C_{p,m}$ and $C_{p,r}$). Explicitly, the relation is:

$$\overline{M}_a^o = \frac{C_{p,m}(T_m^o - T_{1,m}\overline{T}_{eq}) + \overline{M}_r^o C_{p,r}(T_r^o - T_{1,m}\overline{T}_{eq}) + \Delta h_m(1 - f_m(\overline{T}_{eq})) + \overline{M}_r^o \Delta h_r(1 - f_r(\overline{T}_{eq}))}{C_{p,a}(T_{1,m}\overline{T}_{eq} - T_a^o) + \Delta h_a f_a(\overline{T}_{eq})} \quad (9)$$

Note that $f_a(T)$ is the mass fraction of anatectic melt as a function of temperature *for the bulk composition of the country rock*; $f_m(T)$ and $f_r(T)$ are analogous temperature-dependent productivity functions for pristine magma and recharge melt, respectively. The point is that once the total mass of recharge melt added during the RAFC event, the melt productivity functions and the thermodynamic properties of wallrock, pristine and recharge melts are specified, a unique relationship exists between T_{eq} and M_a^o .

4.4. Geochemical and Thermal Paths

[21] To compute the thermal, trace element and isotopic paths of anatectic melt, cumulates, enclaves and homogenized melt within the composite systems, a set of coupled ordinary nonlinear differential equations expressing conservation of enthalpy, mass, species and isotopic composition is solved. The temperature trajectory of the country rock restite (T_a), the mass of assimilant that partially melts (M_a^*), the mass of homogenized melt within the magma body (M_m), the mass of cumulates (M_{ct}), the mass of enclaves (M_{en}) (provided $T_r^o > T_m$ at the moment of recharge) as well as the concentration of trace elements in melt, cumulates and possible enclaves (C_m , C_{ct} , C_{en}) are computed self-consistently. The composition of radiogenic (ϵ_m) and of oxygen (δ_m) isotopes in melt and cumulates is likewise determined. The independent variable is T_m , and the calculation ends when T_{eq} is reached. We emphasize that T_{eq} must be specified in order to compute the path in temperature-composition space because M_a^o involved in the RAFC process, is a function of T_{eq} .

[22] The model consists of $3 + t + i + s$ differential equations where t is the number of trace elements, i the number of radiogenic isotopic ratios and s the number of stable isotopes considered in the calculation. There are no formal limitations on t , s or i except the patience of the geochemist. Pressure is not accommodated explicitly in the current generation EC-RAFC model although adjustment of liquidus and the solidus temperatures ($T_{1,a}$, $T_{1,m}$, $T_{1,r}$ and T_s) can be made to account for variations in pressure when such variations are quantified and deemed critical to the analysis.

[23] The first differential equation is the differential form of the mass recharge function. For episodic input, this is given by (3). The second differential equation expresses conservation of energy along the path as country rock heats up, partially melts and thermally equilibrates with melt from the magma body, which simultaneously undergoes recharge. Energy conservation leads to a differential expression for T_a as a function of T_m . Anatectic melt, generated when wallrock temperature exceeds the solidus, is assumed to rapidly

homogenize with standing magma. It is possible to allow for incomplete extraction of anatectic melt from wallrock by introduction of an extraction efficiency factor (χ). In the current version of EC-RAFC, we assume that all anatectic melt enters the magma body (i.e., $\chi = 1$).

[24] For cases where T_{eq} is less than $T_{1,a}$, the thermal equilibrium condition is $T_a = T_m = T_{\text{eq}}$. When $T_{\text{eq}} > T_{1,a}$, the equilibrium condition is $T_m = T_{\text{eq}}$ since wallrock is completely melted (i.e., $M_a^o = M_a^*$). Recharge melt enters the magma body at T_r^o . The fate of recharge melt depends on T_m . If $T_r^o > T_m$, then because recharge is *assumed* to be intruded at *its* liquidus, a fraction of the recharge melt will crystallize to form enclaves. The fraction of recharge that quenches is given by $1 - f_r(T_m)$ and the mass of enclaves that form is $dM_{\text{en}} = [1 - f_r(T_m)] dM_r$. Enclaves are not in isotopic or trace element equilibrium with standing melt and are distinct from cumulates formed by fractional crystallization of homogeneous standing melt. That fraction of recharge melt which does not “quench” mixes with standing magma and delivers its excess heat to wallrock. In this way, there is an intimate connection between recharge and contamination, a phenomenon considered in more detail below. If, on the other hand, $T_r^o < T_m$ at the time of intrusion, heat is extracted from standing magma and added to the recharge melt. This can give rise to a “wave” of cumulate formation and puts limits on the extent of anatexis.

[25] The differential equation expressing conservation of energy that incorporates the above features gives the derivative of the wallrock (restite) T_a with respect to the T_m along the EC-RAFC path to thermal equilibrium at T_{eq} :

$$\frac{dT_a}{dT_m} = \left(\frac{-1}{\bar{M}_a^o} \right) \cdot \frac{T_{l,m}C_{p,m} + \Delta h_m f'_m(\bar{T}_m) + \bar{M}_a^o C_{p,a} T_{l,m} f_a(\bar{T}_a)}{T_{l,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{l,m}(\bar{T}_m - \bar{T}_a)) f'_a(\bar{T}_a)} + \frac{T_{l,m}C_{p,r} + \Delta h_r f'_r(T_m) \bar{M}_r(\bar{T}_m)}{T_{l,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{l,m}(\bar{T}_m - \bar{T}_a)) f'_a(\bar{T}_a)} + \frac{(T_{l,m}C_{p,r}(\bar{T}_r^o - \bar{T}_m) + (1 - f_r(\bar{T}_m)) \Delta h_r) \frac{d\bar{M}_r}{dT_m}}{T_{l,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{l,m}(\bar{T}_m - \bar{T}_a)) f'_a(\bar{T}_a)} \quad (10)$$

where f'_a and f'_m represent derivatives of the melt productivity functions with respect to T_a and T_m , respectively.

[26] The third constraint is a statement of conservation of total mass. The derivative of the mass of standing melt in the magma body (M_m) with respect to T_m is expressed in terms of the melt productivity functions, their derivatives and the mass recharge function and its derivative with respect to T_m . The mass of melt in the magma body along the path is related to the amount of melt initially present (M_o), the amount added by assimilation of anatectic melt (M_a^*) and by recharge (allowing for enclave formation) and the amount removed by cumulate formation (M_{ct}). The expression has the differential form:

$$\frac{d\bar{M}_m}{dT_m} = \bar{M}_a^o f'_a(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} + f'_m(\bar{T}_m) + f'_r(\bar{T}_m) \bar{M}_r(T_m) + f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \quad (11)$$

Primes on f_a , f_m and f_r denote temperature derivatives.

[27] Conservation of species provides the basis for determining trace element abundances in melt as a function of T_m . Trace element concentration in country rock, pristine standing melt and recharge melt are C_a^o , C_m^o and C_r^o , respectively. We assume that partial melting of country rock is described by fractional melting so that the concentration of trace element in anatectic melt is given by:

$$C_a = \frac{C_a^o}{D_a} (1 - f_a(\bar{T}_a))^{\left(\frac{1-D_a}{D_a}\right)} \quad (12)$$

where D_a is a function of temperature (see Appendix I in the work of *Spera and Bohrsen* [2001] for details). Additionally, a distinct bulk melt-solid partition coefficient D_m , also dependent upon temperature, is defined to account for fractionation of trace element between cumulates and melt. In the enclaves, the distribution of trace element takes place by closed system fractional crystallization of pristine recharge melt. Chilling of a portion of recharge melt by cooler standing magma precludes significant chemical mixing between standing magma and enclaves. The trace element bulk distribution coefficient that describes

the fractionation of a trace element between recharge melt and enclaves is D_r , which generally is temperature-dependent. With these expressions, the species balance expression for the variation of the concentration of trace element in the standing melt as a function of T_m is:

$$\begin{aligned} \frac{d\bar{C}_m}{dT_m} = & \frac{1}{M_m} \left\{ \bar{M}_a^o (s\bar{C}_a - \bar{C}_m) f'_a(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} \right. \\ & + \bar{C}_m (D_m - 1) (f'_m(\bar{T}_m) + \bar{M}_r(\bar{T}_m) f'_r(\bar{T}_m)) \\ & \left. + t (f_r(\bar{T}_m)^{D_r-1} - \bar{C}_m) f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \right\} \quad (13) \end{aligned}$$

The species balance equation accounts for the generation of enclaves as well as cumulates and the introduction of anatectic melt derived by fractional fusion of the assimilated.

[28] For an isotopic ratio in the standing melt ϵ_m , the differential equation is:

$$\begin{aligned} \frac{d\epsilon_m}{dT_m} = & \frac{1}{M_m} \left\{ s \frac{\bar{C}_a}{C_m} (\epsilon_a^o - \epsilon_m) \bar{M}_a^o f'_a(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} \right. \\ & \left. + \frac{t}{\bar{C}_m} ((f_r(\bar{T}_m))^{D_r-1} (\epsilon_r^o - \epsilon_m)) f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \right\} \quad (14) \end{aligned}$$

where ϵ_a^o , ϵ_r^o and ϵ_m represent the isotopic ratio of anatectic melt (identical to wallrock), recharge melt and standing melt at T_m , respectively. Radiogenic in-growth and temperature-dependent isotopic fractionation are neglected in (14). Isotopic equilibrium is assumed to prevail between cumulates and melt; enclaves, on the other hand, are assumed to be in isotopic equilibrium with pristine recharge melt of initial isotopic composition ϵ_r^o .

[29] Finally, the differential equation expressing the oxygen isotope balance in standing melt is:

$$\begin{aligned} \frac{d\delta_m}{dT_m} = & \frac{1}{M_m} \left\{ (\delta_a^o - \delta_m) k_{oxy} \bar{M}_a^o f'_a(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} \right. \\ & \left. + (\delta_r^o - \delta_m) \frac{\Lambda_{r,oxy}}{\Lambda_{m,oxy}} f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \right\} \quad (15) \end{aligned}$$

Temperature-dependent oxygen fractionation is neglected in (15). This effect is generally small at high temperature in magmatic systems (one or two per mil). In cases where magma and country rock

have nearly the same oxygen isotopic ratio, temperature effects may be important and (15) should be modified to include temperature-dependent oxygen isotope fractionation. The ratio $\Lambda_{r,oxy}/\Lambda_{m,oxy}$ represents the mass fraction ratio of oxygen in pristine recharge melt and pristine magma. The mass fraction of oxygen in most natural compositions is about 47% and varies relatively little.

[30] In addition to the primary variables computed by solution of the differential equations, a number of other quantities may be calculated. These are useful because petrologic information is sometimes available for cumulates, enclaves and anatectic melt. The mass, trace element and isotopic composition (path average and instantaneous) of all solids and of anatectic melt along the thermal equilibration path $T_m^o \rightarrow T_{eq}$ may be calculated and compared with available petrologic data. These auxiliary quantities are part of the RAFC solution. Expressions for these quantities are given in the Appendix A.

[31] Equations (3), (10), (11), (13), (14), and (15) constitute a set of $3 + t + i + s$ ordinary differential equations posed as an initial value problem with T_m as the independent variable. This set of coupled differential equations is subject to the following initial conditions: at $T = T_m^o$, $T_a = T_a^o$, $T_r = T_r^o$, $M_m = M_o$, $C_m = C_m^o$ and $C_r = C_r^o$ for t trace element species, $\epsilon_m = \epsilon_m^o$ and $\epsilon_r = \epsilon_r^o$ for i isotope species and $\delta_m = \delta_m^o$ and $\delta_r = \delta_r^o$ for oxygen. The system of differential equations is numerically solved by a fourth-order Runge-Kutta method once cast into dimensionless form. Details of the derivation of the EC-RAFC equations and auxiliary relations are given in the Appendix A.

5. Conclusions

[32] The geochemical evolution of a lithospheric magmatic system is intimately connected to the heat and material exchange between the magma body and its local surroundings. Open system behavior including assimilation of anatectic melts, addition of recharge melt to standing melt (including the formation of chilled solids termed enclaves in EC-RAFC) and cumulate formation by fractional crystallization is more the rule than the exception. Even cursory study of the voluminous

literature on modern and ancient magmatic systems indicates that closed system behavior is uncommon and perhaps even rare. In the EC-RAFC formulation, the processes of melt replenishment, with possible formation of enclaves, assimilation, and cumulate formation are formulated as a set of differential equations with magma temperature as the independent variable. These differential equations express energy, mass, trace element and isotope ratio conservation self-consistently. The EC-RAFC model is flexible and may be applied to any magmatic system independent of its specific three-dimensional configuration provided certain initial conditions and thermodynamic properties are known or can be estimated [e.g., *Spera*, 2000]. In addition to the thermal history and masses of melt, cumulates, enclaves and anatectic contaminants, the EC-RAFC model predicts trace element and isotopic ratios for melt, cumulates, enclaves, and anatectic liquid during RAFC evolution. Although the EC-RAFC model is a simplification of complex petrologic reality, it provides a means to self-consistently model the set of interactions that define the trace element and isotopic evolution of magma chamber melt, associated solids and anatectic liquids. Predicted results can be compared to geochemical data on natural systems in an effort to sharpen our incomplete understanding of the multiphase and multi-component evolution of magmatic systems. In a companion paper [*Bohrson and Spera*, 2002], the EC-RAFC is applied to several petrological problems of interest.

Appendix A

A1. Integral Energy Balance

[33] The model posits that the enthalpy required for heating and partial melting of country rock (heat absorbed) is balanced by the heat liberated by cooling and solidification of melt and solids (cumulates and enclaves). Application of energy conservation provides a relationship between total mass of country rock (M_a^o) and equilibration temperature (T_{eq}) once thermodynamic parameters, initial conditions and the mass of recharge material (M_r^o) added to the standing magma body during

RAFC are specified. In the EC-RAFC formulation, distinct specific isobaric heat capacities and latent heats parameters are distinguished for standing magma, recharge melt and anatectic liquid ($C_{p,m}$, $C_{p,r}$, $C_{p,a}$, Δh_m , Δh_r , Δh_a , respectively). The integral expression for heat liberated is:

$$h_{lib} = M_o C_{p,m} (T_m^o - T_{eq}) + M_o (1 - f_m(T_{eq})) \Delta h_m + M_r^o C_{p,r} (T_r^o - T_{eq}) + M_r^o (1 - f_r(T_{eq})) \Delta h_r \quad (A1)$$

Enthalpy is absorbed by country rock of mass M_a^o as it heats up and undergoes partial fusion, provided the local country rock temperature (T_a) exceeds the solidus (T_s). The initial temperature of country rock is T_a^o , and the entire mass is brought to the equilibration temperature T_{eq} . The fraction of partial melt in the country rock is defined by the melt productivity function $f_a(T)$, which is analogous to $f_m(T)$ and $f_r(T_m)$ defined in the text. The mass of anatectic melt, a quantity that grows during the EC-RAFC event, is defined as M_a^* . The heat of fusion (Δh_a) required for melting is taken as a constant. The integral expression for the heat absorbed by country rock becomes:

$$h_{abs} = M_a^o C_{p,a} (T_{eq} - T_a^o) + f_a(T_{eq}) M_a^o \Delta h_a \quad (A2)$$

By equating the total heat liberated to the heat absorbed, the total mass of country rock, M_a^o , that thermally equilibrates with mass M_o of magma is determined as a function of T_{eq} :

$$\bar{M}_a^o = \frac{C_{p,m} T_{l,m} (\bar{T}_m^o - \bar{T}_{eq}) + \Delta h_m (1 - f_m(\bar{T}_{eq})) + \bar{M}_r^o C_{p,r} T_{l,m} (\bar{T}_r^o - \bar{T}_{eq}) + (1 - f_r(\bar{T}_{eq})) \Delta h_r \bar{M}_r^o}{C_{p,a} T_{l,m} (\bar{T}_{eq} - \bar{T}_a^o) + f_a(\bar{T}_{eq}) \Delta h_a} \quad (A3)$$

It is convenient to use both dimensional and nondimensional terms in the expressions. Recall that that M_o is the mass of magma at T_m^o at the start of the EC-RAFC event and that M_r^o is the total mass of recharge added to the magma body subsystem between T_m^o and T_{eq} . $T_{l,m}$ is used to nondimensionalize the wallrock, standing melt and recharge melt temperature (T_a , T_m , and T_r^o , respectively). Concentrations are scaled to the initial concentrations in magma (C_m^o), wallrock

assimilant (C_a^o) and recharge melt (C_r^o), respectively. The mass of melt (M_m) is scaled by M_o which also is used to scale M_a^o , M_a^* and M_r^o .

A2. Geochemical and Thermal Path

[34] Recharge melt can be either a source (if $T_r^o > T_m$) or sink (if $T_r^o < T_m$) of enthalpy. Enclaves form only in the former case. The mass of enclaves is:

$$M_{en} = \int_{T_m^o}^{T_{eq}} M_r'(T_m)(1 - f_r(T_m))dT_m \quad (A4)$$

The total mass of cumulates (M_{ct}) is:

$$M_{ct} = \int_{T_m^o}^{T_{eq}} -f_r'(T_m)\bar{M}_r(\bar{T}_m)d\bar{T}_m - \int_{T_m^o}^{T_{eq}} f_m'(\bar{T}_m)d\bar{T}_m \quad (A5)$$

The primes in the above expressions mean that derivatives with respect to T_m have been taken. The total mass of all solid products generated during a RAFC event (M_s) is given by $M_s = M_{en} + M_{ct}$ using (A4) and (A5).

[35] Once M_a^o has been computed algebraically from (A3), the differential equations defining the geochemical and thermal paths may be solved. Energy conservation for each step along the EC-RAFC path enables determination of wallrock restite temperature (T_a) as a function of T_m . We adopt the convention that absorbed heat is positive. Energy conservation demands that $h_{lib} + h_{abs} = 0$; differentiation with respect to T_m , application of the chain rule and rearrangement give the following for the variation of T_a with respect to T_m :

$$\frac{d\bar{T}_a}{dT_m} = -\left(\frac{dh_{lib}/d\bar{T}_m}{dh_{abs}/d\bar{T}_a}\right) \quad (A6)$$

The differential forms for liberated and absorbed enthalpies are:

$$\begin{aligned} \frac{dh_{lib}}{dT_m} = & -\frac{1}{M_o} (T_{1,m}C_{p,m} + \Delta h_m f_m'(\bar{T}_m) + \bar{M}_a T_{1,m}C_{p,a} f_a'(\bar{T}_a) \\ & + (T_{1,m}C_{p,r} + \Delta h_r)\bar{M}_r(\bar{T}_m) + (T_{1,m}C_{p,r}(\bar{T}_m - \bar{T}_r^o) \\ & + (f_r(\bar{T}_m) - 1)\Delta h_r) \frac{d\bar{M}_r}{dT_m} \end{aligned} \quad (A7a)$$

and

$$\begin{aligned} \frac{dh_{abs}}{dT_a} = & M_o \bar{M}_a^o (T_{1,m}C_{p,a}(1 - f_a(\bar{T}_a)) \\ & + (T_{1,m}C_{p,a}(\bar{T}_m - \bar{T}_a) + \Delta h_a) f_a'(\bar{T}_a)) \end{aligned} \quad (A7b)$$

Substitution of (A7a) and (A7b) in (A6) gives the required expression written in nondimensional form:

$$\begin{aligned} \frac{d\bar{T}_a}{dT_m} = & \left(\frac{-1}{\bar{M}_a^o}\right) \\ & \cdot \frac{T_{1,m}C_{p,m} + \Delta h_m f_m'(\bar{T}_m) + \bar{M}_a^o C_{p,a} T_{1,m} f_a'(\bar{T}_a)}{T_{1,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{1,m}(\bar{T}_m - \bar{T}_a)) f_a'(\bar{T}_a)} \\ & + \frac{T_{1,m}C_{p,r} + \Delta h_r f_r'(T_m)\bar{M}_r(\bar{T}_m)}{T_{1,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{1,m}(\bar{T}_m - \bar{T}_a)) f_a'(\bar{T}_a)} \\ & + \frac{(T_{1,m}C_{p,r}(\bar{T}_r^o - \bar{T}_m) + (1 - f_r(\bar{T}_m))\Delta h_r) \frac{d\bar{M}_r}{dT_m}}{T_{1,m}C_{p,a}(1 - f_a(\bar{T}_a)) + (\Delta h_a + C_{p,a} T_{1,m}(\bar{T}_m - \bar{T}_a)) f_a'(\bar{T}_a)} \end{aligned} \quad (A8)$$

By convention Δh_a , Δh_m and Δh_r are positive numbers and primes denote differentiation with respect to T_m or T_a as appropriate. T_a is computed so long as $T_a < T_{1,a}$; for $T_a \geq T_{1,a}$ wallrock is entirely molten and the relevant equilibrium condition is $T_m = T_{eq}$. Conservation of mass gives rise to a differential form for the variation of the mass of melt within the magma body (M_m) with melt temperature T_m :

$$\begin{aligned} \frac{d\bar{M}_m}{dT_m} = & \bar{M}_a^o f_a'(\bar{T}_a) d\bar{T}_a d\bar{T}_m + f_m'(\bar{T}_m) + f_r'(\bar{T}_m)\bar{M}_r(T_m) \\ & + f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \end{aligned} \quad (A9)$$

Expression (A9) accounts for the addition of anatectic melt and the appropriate fraction of recharge melt as well as the removal of mass by cumulate and enclave formation along the EC-RAFC path. The last two terms on the RHS of (A9) account for changes in the mass of melt within the magma body due to recharge. Since some of the recharge melt may chill to form enclaves and some of it may remain liquid, it is necessary to include the temperature derivative of the recharge melt productivity function.

[36] Trace element conservation enables one to write a differential equation for the concentration

of trace element in the melt as a function of T_m . This balance models addition of trace element into melt due to partial melting (fractional fusion) of country rock and magma recharge as well as removal of trace element by fractional crystallization of cumulates. Enclaves are assumed to form wholly from pristine recharge melt and do not affect the composition of standing melt. The fraction of recharge mass that does not freeze to form enclaves (i.e., recharge melt at T_m) homogenizes with standing magma. For partial melting in wallrock, we assume fractional melting occurs. The concentration of trace element in anatectic liquid at T_a is:

$$C_a = \frac{C_a^o}{D_a} (1 - f_a(\bar{T}_a))^{\frac{1-D_a}{D_a}} \quad (\text{A10})$$

where D_a is the distribution coefficient (the equilibrium constant of the trace element distribution reaction) between anatectic melt and residual restitic wallrock. The average concentration of trace element of anatectic melt delivered to the evolving magma body in the temperature interval $T_a^o \rightarrow T_a$ is:

$$\hat{C}_a = \frac{C_a^o}{f_a(T_a)} \left[1 - (1 - f_a(T_a))^{1/D_a(T_a)} \right] \quad (\text{A11})$$

The concentration of trace element available for mixing into standing magma differs from that in pristine recharge melt because of depletion or enrichment due to enclave crystallization. This process is modeled as closed system fractional crystallization according to:

$$C_r = C_r^o [f_r(T_m)]^{D_r-1} \quad (\text{A12})$$

In (A12), C_r represents the trace element concentration in residual recharge melt after enclave formation, C_r^o is the concentration of trace element in pristine recharge melt and D_r is the partition coefficient between enclave and recharge melt. All trace element equilibrium constants are taken as functions of temperature:

$$D_a = D_a^o \exp\left(\frac{-\Delta H_a}{RT_{l,m}} \cdot \frac{1}{\bar{T}_a}\right) \quad (\text{A13a})$$

$$D_m = D_m^o \exp\left(\frac{-\Delta H_m}{RT_{l,m}} \cdot \frac{1}{\bar{T}_m}\right) \quad (\text{A13b})$$

$$D_r = D_r^o \exp\left(\frac{-\Delta H_r}{RT_{l,m}} \cdot \frac{1}{\bar{T}_m}\right) \quad (\text{A13c})$$

In (A13), ΔH_j with $j \in \{a, m, r\}$ represent the effective enthalpies of the reactions governing bulk partitioning of trace element between anatectic melt and country rock restite, standing melt and cumulates, and pristine recharge melt and enclaves, respectively. The ΔH_j values are “effective” values in the sense that the dependence of D_j on phase assemblage is parameterized implicitly using the temperature dependence of D_j . That is, “effective” values ΔH_j are chosen by consideration of phase equilibria relevant to the bulk compositions and equilibrium phase assemblages of $\{a, m$ and $r\}$ along the temperature trajectory $T_m^o \rightarrow T_{eq}$. If this auxiliary information is not available or poorly known, constant bulk partition coefficients D_j may be used by setting ΔH_j equal to zero. With these auxiliary relations, trace element conservation in the melt (C_m) is expressed as follows:

$$\begin{aligned} \frac{d\bar{C}_m}{d\bar{T}_m} = \frac{1}{\bar{M}_m} \left\{ \bar{M}_a^o (s\bar{C}_a - \bar{C}_m) f'_a(\bar{T}_a) \frac{d\bar{T}_a}{d\bar{T}_m} \right. \\ \left. + \bar{C}_m (D_m - 1) (f'_m(\bar{T}_m) + \bar{M}_r(\bar{T}_m) f'_r(\bar{T}_m)) \right. \\ \left. + t (f_r(\bar{T}_m)^{D_r-1} - \bar{C}_m) f_r(\bar{T}_m) \frac{d\bar{M}_r}{d\bar{T}_m} \right\} \quad (\text{A14}) \end{aligned}$$

where $s = C_a^o/C_m^o$ and $t = C_r^o/C_m^o$.

[37] Once the concentration of trace element in standing melt is known, trace element concentrations in cumulates and enclaves may be determined. EC-RAFC computed compositions provide a relative chronology of the cumulates produced during the RAFC event. Similarly, the trace element composition of enclaves will also vary during the RAFC event.

[38] The instantaneous concentration of a trace element in enclave (at $T = T_m$) is:

$$C_{en} = C_r^o D_r [f_r(\bar{T}_m)]^{D_r-1} \quad (\text{A15})$$

whereas the average trace element concentration in enclaves along the path $T_m^o \rightarrow T_m$ is:

$$\hat{C}_{en} = \frac{C_r^o [1 - f_r^{D_r}(\bar{T}_m)]}{(1 - f_r(T_m))} \quad (\text{A16})$$

The instantaneous concentration of trace element in cumulate at T_m is given by:

$$C_{ct} = C_m^o \bar{C}_m D_m \quad (A17)$$

where \bar{C}_m is calculated in (A14). The average trace element composition in all cumulates formed along the path $T_m^o \rightarrow T_{eq}$ is:

$$\hat{C}_{ct} = \frac{C_m^o D_m \left[\int_{T_m^o}^{T_{eq}} f_r(\bar{T}_m) M_r(\bar{T}_m) \bar{C}_m dT_m + \int_{T_m^o}^{T_{eq}} f_m(\bar{T}_m) \bar{C}_m dT_m \right]}{\int_{T_m^o}^{T_{eq}} f_r(\bar{T}_m) M_r(\bar{T}_m) dT_m + \int_{T_m^o}^{T_{eq}} f_m(\bar{T}_m) dT_m} \quad (A18)$$

[39] The isotopic evolution of melt is calculated by neglecting radiogenic ingrowth and assumes isotopic equilibrium between magma body melt and cumulates. Upon generation, anatectic melt is assumed to be in isotopic equilibrium with country rock and thereafter to mix thermally, chemically and isotopically with melt in the standing magma body. The fate of recharge melt depends upon T_m and T_r^o . It is assumed that recharge melt is injected at its liquidus temperature. At the instant of intrusion, the fraction of recharge that chills to form enclaves is given by the recharge melt productivity function. That portion of the recharge material that does not solidify is allowed to homogenize chemically, isotopically and thermally with standing melt. The isotope balance expression that incorporates these features is:

$$\frac{d\varepsilon_m}{dT_m} = \frac{1}{M_m} \left\{ s \frac{\bar{C}_a}{C_m} (\varepsilon_a^o - \varepsilon_m) \bar{M}_a f_a'(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} + \frac{t}{C_m} ((f_r(\bar{T}_m))^{D_r-1} (\varepsilon_r^o - \varepsilon_m) f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m}) \right\} \quad (A19)$$

where ε_a^o , ε_r^o and ε_m represent the isotopic ratio of anatectic melt, pristine recharge melt and standing melt, respectively.

[40] The oxygen isotope balance is computed neglecting temperature dependent isotopic effects. For lighter isotopes, such as D/H, thermal fractionation is important and (A20) would have to be modified. Even for oxygen there is a small (\sim several per mil) temperature fractionation effect

that should be kept in mind. However, in most situations, the significantly different oxygen isotopic composition of country rock and melt (standing or recharge) overwhelms thermal fractionation effects. The form of the balance becomes:

$$\frac{d\delta_m}{dT_m} = \frac{1}{M_m} \left\{ (\delta_a^o - \delta_m) k_{oxy} \bar{M}_a f_a'(\bar{T}_a) \frac{d\bar{T}_a}{dT_m} + (\delta_r^o - \delta_m) \frac{\Lambda_{r,oxy}}{\Lambda_{m,oxy}} f_r(\bar{T}_m) \frac{d\bar{M}_r}{dT_m} \right\} \quad (A20)$$

where δ_a^o , δ_r^o and δ_m represent the oxygen isotope composition (conventional nomenclature) of anatectic, recharge and standing melt, respectively. The quotients $\Lambda_{a,oxy}/\Lambda_{m,oxy}$ and $\Lambda_{r,oxy}/\Lambda_{m,oxy}$ represent the mass fraction ratio of oxygen in assimilant and pristine melt and recharge and pristine melt, respectively. Except for rare bulk compositions such as carbonatites or other, extremely silica-undersaturated compositions these ratios are generally quite close to unity. Equations (A8), (A9), (A14), (A19), (A20), and (3) represent a system of differential equations with T_m as the independent variable. This set of coupled nonlinear ordinary differential equations is of order $3 + t + i + s$ where t is the number of trace elements, i is the number of radiogenic isotope ratios and s is the number of stable isotope ratios in the calculation. In order to solve the EC-RAFC differential equations, initial conditions must be specified. A typical set of initial conditions (in dimensional terms) is as follows: at $T_m = T_m^o$, let $T_a = T_a^o$, $T_r = T_r^o$, $M_m = M_o$, $C_m = C_m^o$, $\varepsilon_m = \varepsilon_m^o$, $\varepsilon_a = \varepsilon_a^o$, $\varepsilon_r = \varepsilon_r^o$, $\delta_m = \delta_m^o$ and $\delta_a = \delta_a^o$. The system of ordinary differential equations is solved numerically by a fourth-order Runge-Kutta method with fixed step size. A coarse step size of 0.001 is suggested for exploratory work. Once a set of parameters has been refined, the step size should be serially decreased by a factor of two until computed variables (e.g., T_a , M_m , C_m , ε_m , ε_a , δ_a , δ_m , etc) no longer change with step size. When this limit is reached, the solution may be considered converged and precise. In general, small step sizes should be used if D_a , D_m or $D_r \gg 1$. A complete solution takes tens to hundred to thousands seconds on a 500 MHz machine

depending on the step size and the number of trace elements and isotope ratios computed. For information about the availability of downloadable EC-RAFC code, go to <http://magma.geol.ucsb.edu/>. A computer code for EC-AFC is available at the same website.

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