

Elements of a modeling approach to the physical controls on crustal differentiation

G. W. BERGANTZ AND S. A. BARBOZA

14.1 Introduction

Crustal differentiation is a progressive, and sometimes repeated, process of phase change, transport, and emplacement (Brown, 1994). For example, the upward migration of melts depleted in Y and the heavy rare earth elements (HREEs), which are generated during high-grade metamorphism, tends to stratify the concentration of large ion lithophile elements within the crust, concentrating them in the upper crust (Chapter 4). However, as with many persistent issues in crustal differentiation, the appropriate length scales of the compositional gradients and rates of the transport processes are unknown.

The essential process in crustal differentiation is the relative motion between phases; without relative motion there will be no differentiation, only bulk transport. Advective processes govern crustal-scale differentiation, as diffusion is not capable of transporting sufficient mass, but there are a number of questions that remain unanswered about these processes. What are the controls on relative motion? What are the mechanics of phase gathering and dispersal? To what degree are putative thermodynamic volumes controlled by rheological contrasts and reaction rates? All geological flow is formally chaotic in the sense of Aref (1990) and Ottino (1989), and includes crossing scales of influence (Petford *et al.*, 1997; Brown & Solar, 1998a, b; Yuen *et al.*, 2000), but are there underlying simplifications that are useful for geological applications?

Relatively simple, but interrelated, deterministic laws for which the dynamics may be quite complex govern geological systems. This yields systems possessing a dual nature; there is a tendency to disorder, but that is offset by the underlying mechanical deterministic templates. It is our view that these deterministic templates reflect multiphase, multiscale processes. Our objective in this final chapter is to review modeling strategies for addressing the

transport mechanics of these multiphase, multiscale processes and to offer guidelines and recommendations for their quantitative assessment.

When coupled with deterministic models, both ergodic theory and chaotic dynamics provide possible approaches to constructing explanations that may bridge the heterogeneous scales of the information content of natural examples. Our emphasis is largely on the fluid-dominated regime of crustal differentiation; we will not discuss physical processes that have been addressed adequately elsewhere (e.g., Holness, 1997) and in earlier chapters. Hence, we will focus on methodologies and physical considerations that have not been elaborated previously, and that the student of crustal processes may find of some use.

One new but widely applied paradigm for multiphase systems invokes the notion of “granularity.” In the broadest sense, granularity refers to the structure of the information content of a data set. It may also refer to the indeterminacy, or limits of resolution, of both space and time in a data set. Granularity in our context refers to the hierarchy of size, or scale, or levels of detail, that is intrinsic to geological data sets. It is important to appreciate that spatial granularity scales, such as the size, composition, and distribution of leucosomes in a migmatite, may have very different temporal granularity. Thus, the definition of proximity may take on different scales in both space and time.

This is implicit in the recognition that the geological systems that lead to crustal differentiation are open systems, and that the information content of an outcrop may exhibit deformation of both spatial and temporal elements. For example, a leucosome may be the result of intermittent melt migration and the composition may not reflect any simple relationship to the surrounding melanosome (e.g., Sawyer, 1999), or the thickness of a dike while magma is flowing may be greater than the measured thickness in the field, or the thermal conditions during partial melting may be overprinted by subsequent high-temperature events. Other examples include the plutonic expression of magma mixing and mingling, where what one observes in the field is the complex superposition of events that represent the very last and least dynamic state of the system (e.g., Bergantz, 2000). Thus, geological samples may be “over-sampled” with respect to temporal, kinematic, or compositional information in a way that is difficult to assess.

Data granularity is an explicit expression of phase-relative motion and, hence, multiphase processes. Each of these processes has characteristic length and time scales, and it is the nonlinear interactions and feedback among them that give rise to the dissipative structures that are recorded as spatial variations in composition and kinematic character of a rock body. These elements compose the “memory” of a rock body, and the spatial distribution of “memory” is not likely to be linearly related to time, especially in bodies with

isotherms that are associated with profound rheological transitions (e.g., Vigneresse *et al.*, 1996).

14.2 Some general principles of multiphase flow

Practically all geological systems are multiphase, multicomponent systems. A phase is a physically distinct portion of matter, and a mixture is any multiphase ensemble. For example, magma may be composed of numerous solid phases, a melt phase and perhaps a separate volatile phase, all of which may move with non-zero phase and relative velocities. If the melt phase is volumetrically dominant, it would be called the “carrier phase,” and we might consider the mixture a dilute suspension. This simplifies the physical description of the multiphase mixture considerably, as the interphase coupling is not important in describing the bulk flow. The other extreme would be flow through a fixed porous medium, in which the velocity of the solid phase usually is taken to be small or zero and the velocity of the fluid phase is non-zero. In this case, the solid phase is volumetrically dominant. Developing a continuum description of multiphase heat and mass transfer for all possible conditions, from melt to solid dominated, has been especially challenging due to the change in the intrinsic averaging scales that define the continuum.

14.3 Suspensions and slurries

14.3.1 Definitions

It is apparent that a dispersed-phase mixture is not a continuum in the molecular limit, and one must develop carefully the definition of a material “point” so that the differential equations of transport may be applied to the mixture (Poletto & Joseph, 1995). The definition of mixture quantities requires the definition of a stationary average volume ΔV_o .

$$\Delta V_o = N_m L^3, \quad (14.1)$$

where N_m is the minimum number of particles for a stationary average, and L is the particle spacing. If L is taken to be 10 particle diameters, the particle diameters to be 0.5 mm and N_m to be 10^3 , the stationary average volume ΔV_o is 0.125 m^3 , or a volume 0.5 m on a side. If this dimension is of the same order of magnitude of the system scale, defined to be the scale that describes some distinct region of homogeneity, then the mixture cannot be treated as a continuum. Considering that many migmatite bodies have measurable variability at or below this scale, attempts to integrate kinematic and compositional

elements with continuum theory require considerable care. Equation (14.1) provides a measure of what might be considered geological “noise” relative to a model that represents averaged quantities, and highlights the difficulties of invoking the continuum assumption for many geological applications.

Equation (14.1) motivates the definition of the phase volume fraction, ε_p :

$$\varepsilon_p = \lim_{\Delta V \rightarrow \Delta V_0} \frac{\Delta V_p}{\Delta V} \tag{14.2}$$

for a phase volume of ΔV_p . Conservation of mass requires that the volume fraction of n phases sum to unity

$$\sum_{i=1}^n \varepsilon_i = 1. \tag{14.3}$$

The mechanics of the relative motion between melt, cumulate, and residual phases determine the length and time scales of crustal differentiation. Such mixtures are described as suspensions or slurries, depending on the degree to which the presence of particles influences the rheology or the exchange of momentum (Roberts & Loper, 1987; Marsh, 1988; Iverson, 1997). The mechanics of a dilute suspension are governed largely by the physical properties of the melt. With increasing solid fraction, the suspension may undergo a transition to a slurry, the mechanics of which are dominated by the transmission of stress and/or momentum between the separate phases. Kinematic and dynamic criteria provide alternative quantitative definitions for the suspension to slurry transition.

The kinematic criterion follows from the rule-of-thumb that particles that are closer than two to three diameters experience mutual hydrodynamic interaction and so cannot be considered to be isolated elements, and so the mixture is not a dilute suspension. One implication of this is that simple drag laws, such as Stokes’ law are not applicable without some correction. If it is assumed that the particles are equally spaced, the particle diameter, D , the particle spacing, L , and the volume fraction are related by

$$\frac{L}{D} = \left(\frac{\pi}{6\varepsilon_p} \right)^{1/3}, \tag{14.4}$$

and so for a particle volume fraction of 0.1, the particle spacing ratio is about 1.7, and the particles cannot be treated as individual elements. Therefore, the mechanics of a multiphase mixture is influenced by particle collisions or hydrodynamic interactions even at particle volume fractions of less than 10%, and the multiphase mixture cannot be considered as a simple collection of single particles.

A highly simplified dynamic criterion for the suspension-to-slurry transition may be obtained by the consideration of whether the mixture is dilute or dense. In a dilute mixture, the momentum transfer is strictly between the particle and the drag and lift forces of the fluid, and particle–particle interactions are negligible. One measure of mechanical dilution is the particle response time. The particle response time is the time necessary for the fluid to influence the particle trajectory. For example, if the particle response time to the fluid forces is shorter than the time between particle collisions, the fluid is dilute because particles are dominantly responding to fluid forces. Conversely, if the particle–particle collisions happen so rapidly that the particle cannot respond to fluid forces before the next collision, the fluid is considered to be a slurry.

The particle response time τ_M to the fluid forces in the particle sub-inertial or Stokes regime range (note that the fluid may still be turbulent), is given by (Marble, 1970; Crowe *et al.*, 1996)

$$\tau_M = \frac{\Delta\rho D^2}{18\mu}, \quad (14.5)$$

where $\Delta\rho$ is the particle–fluid density contrast, D the particle diameter and μ the dynamic viscosity of the carrier phase. The time between particle collisions is

$$\tau_C = \frac{1}{n\pi D^2 \nu_r}, \quad (14.6)$$

where n is the number density of particles, and ν_r the relative velocity between particles. Thus, the requirement for a mixture to be dilute is

$$\frac{\tau_M}{\tau_C} \quad (14.7)$$

For a relative velocity of unity, which is probably much higher than what one might have in practice, and the relatively high viscosities, the criterion for a dilute condition might be satisfied even to high particle volume fractions in most geological applications. A more complete dimensional and scaling analysis of momentum transport at high particle volume fraction provides additional dynamic criteria for distinguishing multiphase flow regimes (Iverson, 1997).

14.3.2 Characteristic scales of crystal sorting and sedimentation

Many expressions of transport of multiphase mixtures may be addressed by consideration of the particle momentum response time. The equation

of motion for a non-steady, single particle is given by the Basset–Boussinesq–Oseen equation (BBO), which is a complex integro-differential equation (Stock, 1996; Kim *et al.*, 1998). However, if one is interested in the time-averaged behavior, and if the fluctuations in the flow-field are not rapid, many of the complications of the BBO equation may be neglected (Vojir & Michaelides, 1994). With these caveats in mind, we will focus on the (pseudo) steady-state drag term, as the integrated influence of this term dominates the particle–fluid interaction.

First, we introduce the characteristic time scale for the flow

$$\tau_F = \frac{L_O}{U_O}, \quad (14.8)$$

where U_O and L_O are the local characteristic velocity and length scale of the flow (but also see Crowe, 2000). The ratio of the particle response time to the characteristic time scale of the fluid motion is called the Stokes number, Sk , and is given by

$$\frac{\tau_M}{\tau_F} = Sk, \quad Sk = \frac{\Delta\rho D^2 U_O}{18\mu L_O} \quad (14.9)$$

(Ling *et al.*, 1998). If the Stokes number is much less than 1, the particle relaxation time is small relative to the time it experiences the fluid forces, velocity equilibrium will be immediately attained, and the particle dispersion will be the same as the fluid dispersion (Yang *et al.*, 2000). Conversely, if the Stokes number is large, the particles do not have sufficient time to respond to fluid forces, and will move through the flow field without being entrained by the flow. When the Stokes number is near unity, the fluid has sufficient viscosity to spin the particle to significant angular velocities without suppressing the radial trajectory. Thus, the particle relaxation time is matched to the eddy rotation time, and the particles circulate on the margins of the eddy. This provides a mechanism for the de-mixing of an initially well-mixed multiphase fluid, and in fact may lead to particle sorting and selective sedimentation even in turbulent flow (Zarrebini & Cardoso, 1998).

Gravity forces introduce another time scale in the description of the particle motion, which leads to the scaled particle settling time

$$\tau_S = \frac{18\mu L_O}{\Delta\rho D^2 g}, \quad (14.10)$$

which is the time it takes the particle to settle through an eddy of diameter L_O . This time scale provides a partial measure of the time a particle has available

for chemical reaction within a dynamic eddy, the state of which is defined by an average chemical potential. One important difference between the particle response time scale, τ_M and the particle settling time scale, τ_S , is that the particle response time scale represents the time scale of unsteady motions. The particle settling time scale is that associated with the steady forcing of gravity (Raju & Meiburg, 1995; Burgisser & Bergantz, 2002). The ratio of the particle settling time and the scaled flow time is

$$\frac{\tau_S}{\tau_F} = \frac{Fr^2}{Sk}, Fr = \frac{U_0}{\sqrt{L\sigma g}}, \quad (14.11)$$

where Fr is the Froude number. Neglecting some terms for brevity of discussion, the BBO equation may now be written as

$$\frac{d\mathbf{v}_p}{dt} = \frac{f}{Sk} [\mathbf{u}(\mathbf{X}, t)|_{\mathbf{x}=\mathbf{x}_p} - \mathbf{v}_p(t)] + \frac{1}{Fr^2} \mathbf{e}_g, \quad (14.12)$$

where \mathbf{u} is the fluid velocity evaluated at the particle, \mathbf{v}_p the particle velocity, and \mathbf{e}_g the unit direction of the acceleration of gravity. The term, f , provides for departures from Stokes drag at higher-particle Reynolds number, or for more involved corrections related to turbulence intensity, non-spherical particles and other factors.

The notion of particle response time may be extended to heat and mass transfer as well. As with the case of non-steady motion, a complete description of the non-steady heat and mass transfer between a particle and the carrier (fluid) phase yields a complex integro-differential equation (Michaelides & Feng, 1994; Feng & Michaelides, 2000). However, a useful characteristic time scale for the particle thermal response time to changes in the fluid temperature is

$$\tau_T = \frac{\rho_P c_P D^2}{12k_c} \quad (14.13)$$

where ρ_P is the particle density, c_P the particle specific heat capacity and k_c the thermal conductivity of the carrier phase.

14.3.3 Phase segregation by shear

Particle dispersal and gathering takes place in both rectilinear and curvilinear flow at low carrier-phase Reynolds number, where there is little time-dependence to the flow. There are many physical manifestations of this process, such as the resuspension of a particles that have settled, or the migration of particles

out of regions of high shear as observed in conduit and viscometer flow (Karnis *et al.*, 1966; McTigue *et al.*, 1986; Leighton & Acrivos, 1987; Averbakh *et al.*, 1997; Lyon & Leal, 1997; Marchioro & Acrivos, 2001). Two theories have been used to illuminate these physical processes: (1) the Lagrangian approach, such as the Stokesian dynamics (Brady & Bossis, 1988; Singh & Nott, 2000; Marchioro & Acrivos, 2001), or (2) the lattice Boltzmann approach (Aidun *et al.*, 1998), and the effective continuum (non-local) models where the movement of individual particles is represented by changes in the local particle volume fraction.

Of the continuum models, there are generally two approaches to the physical description of the migration of particles: (1) the diffusive flux model of Leighton and Acrivos (1987), subsequently extended by Phillips *et al.* (1992), and (2) the granular “temperature,” or suspension balance models, of Jenkins and McTigue (1990) and Nott and Brady (1994). The diffusive flux model is a phenomenological model that attempts to describe the non-local particle migration perpendicular to the shear plane as a diffusion process, and a constitutive equation is derived for the particle flux. In this model, the shear-induced particle diffusivity is linearly proportional to the local shear rate. The description of particle segregation from the initial inlet conditions to a final steady configuration is given by a particle volume fraction conservation balance, where the particle segregation flux, \mathbf{J} , is explicitly decomposed into contributions from gravitational and hydrodynamic forces, and spatial variations in viscosity as a function of local particle volume fraction (Fang & Phan-Thien, 1995; Subia *et al.*, 1998; Shauly *et al.*, 2000). The explicit forms of the contributions to the general model for the particle segregation \mathbf{J} are complex, and the interested reader is directed to the references given above. Despite the fact that the phenomenological diffusive flux approach is ad hoc, it does provide an accessible, empirically based model for particle migration in simple shear flow that is amenable to numerical implementation.

The granular temperature model of Jenkins and McTigue (1990) is based on the notion of a scalar migration potential associated with just the particle phase. The suspension balance model of Nott and Brady (1994), while also invoking the notion of particle temperature and, hence, pressure, includes both phases. However, both models have been difficult to use and implement. One notable exception is the study of Petford and Koenders (1998), which employs the model of Jenkins and McTigue (1990) to assess the possibility of particle migration in the flow of silicic dikes. However, it has been concluded subsequently that the definition of a granular temperature as a scalar variable is not very realistic, as the particle velocity fluctuations are highly anisotropic (Shapley *et al.*, 2002, 2004). This does not mean that these models have no

utility for geological applications, only that they are currently most useful in the high-Peclet number limit where putative particle temperatures have a negligible contribution to the potential energy of the transport.

An extension of the so-called “suspension balance approach” offers a more fundamental theory of particle segregation (Morris & Boulay, 1999), and does not require ad hoc tuning of field variables as in the diffusion flux model, nor invoke (inspired but) model-based notions such as granular temperature. It is a rheologically based approach, and has the advantage over the diffusive flux model that anisotropy of normal stresses is explicitly modeled and its role as the cause of particle segregation is explained. This approach satisfactorily recovers many of the experimental results, and illuminates how the normal stresses fall-off quadratically as the particle volume fraction becomes small. In fact, it has been difficult experimentally to demonstrate particle migration for very dilute systems where the particle volume fraction is less than 10% (Hampton *et al.*, 1997). Thus, we would expect that particle segregation during flow will be more important at higher solid fraction, such as one might obtain in diatexites. The implementation of the model is rather complicated, and the needed experimental work to provide the transport coefficients for the normal and shear stress rheology and the particle hindrance function has yet to be done.

Of central interest to geological applications is the time scale over which unmixing, or particle migration, may occur. Most theories and experiments predict that the length scale, L , over which an initially well-mixed material will un-mix as a consequence of particle migration, will scale as (Nott & Brady, 1994; Phan-Thien & Fang, 1996; Hampton *et al.*, 1997)

$$L \approx \frac{W^3}{a^2} (1.1), \quad (14.14)$$

where W is the width of the channel, and a is the particle radius. For a diatexite or dike in simple pressure flow (i.e., 0.5 m wide, and a residual particle radius of 5 mm, the length scale to a steady particle profile is 5 km. Thus, despite being in a state of very low Reynolds number, the material being transported will have a complex history. This indicates that assuming steady conditions in the modeling of a multiphase conduit requires some justification. If the channels do not have a simple geometry, although the flow is laminar, it will be chaotic (Jones *et al.*, 1989; Wang *et al.*, 1990). This may complicate the assessment of steady-state conditions further. In addition, all the models described above are for conditions of mono-disperse mixtures, which are unlikely to be the norm in practice. For poly-disperse mixtures, more complex arrangements may result (Shauly *et al.*, 2000), and the first-order physical models are not yet available that include normal stresses.

14.4 Mixing and compositional heterogeneity

One of the most challenging aspects in the study of crustal differentiation is the association of upper-crustal products with their source areas. This is partly a consequence of the fact that these source areas are rarely exposed, but is also due to open-systems processes of differentiation and mixing that produce intermittent homogenization and fractionation, which may mask source area diagnostics. These processes are mixing in the sense that conditions change from one state of simplicity to another (Tavare, 1986). For example, source regions may be regionally simple in the statistical sense of bulk composition, mode, kinematic fabric, etc., and the ultimate product of crustal differentiation (a granite, for example) might manifest similar scales of statistical uniformity. But this simplicity is the result of complex open system processes and dissipative structures, so how may one see through the low-energy final products and characterize the complex spatial and temporal patterns? This motivates us to consider some of the physical controls on the time and space scales of mixing in multiphase reacting flow.

In the discussion below, we consider only mixing that is a consequence of advection. The role of velocity is two-fold, it increases the surface area by stretching, and aids diffusion by transporting folded and stretched elements. We do not explicitly consider the mixing that results from diffusion alone across a solid, bounding body. These are controlled by the diffusivity of compositional elements, which is much less than the thermal diffusivity, which is often rate-controlling. We will also not consider the mixing of granular systems, where the momentum exchange and dissipative structures are dominated by particle–particle friction. These processes have been considered by Khakhar *et al.* (1999), but are not obviously relevant to melt-present advective transport dominated by buoyancy changes in a gravity field.

Mixing may be regarded generally as consisting of three distinct stages: (1) initial interpenetration or injection; (2) stirring, and (3) mixing by molecular diffusion. The interpenetration stage initializes the macroscopic bodies of a composite system with a distinct volume, surface, and position. This stage may also provide for the potential energy for subsequent internal mixing, the initial distribution of surface area, and so transports extensive properties associated with distinct, pre-mixed volumes.

One may imagine two end-members to this process. The first is where the interpenetration process brings pre-mixed volumes together with sharp boundaries. This typically happens if there is a contrast in viscosity and thermophysical properties, and if the Reynolds number is low, which may often be the case in diatexites or dikes (Petford, 1996). This could form distinct

islands of unmixed material, which would then undergo blending by repeated stretching. Another end-member is where the interpenetration process is intimately accompanied by mixing, and the stirring and interpenetration stages are virtually indistinguishable. This is called “stationary entrainment” and requires nearly equal viscosities and the rapid, local, conversion of potential energy to kinetic energy at high Reynolds number conditions, such as that documented by Linden *et al.* (1994). Examples of both end-members are illustrated in the flow of multiphase plumes by Bergantz and Ni (1999).

The dissipative structures that do the work of mixing, such as Taylor layers (Broadwell & Mungal, 1991), are essentially transient and difficult to quantify after the process is completed. In the context of mantle convection there have been significant efforts to elucidate the mixing of passive features (Hoffman & McKenzie, 1985). These modeling efforts demonstrate that the mixing times and time-dependent spatial scales are sensitive to both the kinematics of the flow and the rheology, and are difficult to generalize. For example, models of Rayleigh–Bernard convection under mantle conditions reveal that Newtonian rheology produces more rapid progress to mixing than does a non-Newtonian material (Ten *et al.*, 1997). Forward modeling provides valuable insights into specific conditions of mixing and has significant heuristic value, but does not usually have generic and widespread applicability due to the wide range of possible and chaotic conditions. For example, this approach generally does not relate a general metric of mixing efficiency to a particular velocity field.

This motivates some definitions of the state of mixing, as proposed by Danckwerts (1952) and implemented in a geological context by Oldenburg *et al.* (1989), which is recommended as a succinct introduction. Two measures of mixing are the scale and intensity of segregation, as long as there are no persistent large-scale heterogeneities. The scale of segregation is associated with a two-point correlation function and is related to the average traversal length through the phases. This function gives the probability that two volume elements of a concentration, C , will be correlated

$$R(|\mathbf{r}|) = \frac{\overline{C_i(x+r) \cdot C_i(x)}}{\overline{C_i^2}}, \quad (14.15)$$

where C_i is the deviation from the system average concentration. Note that for large values of $|\mathbf{r}|$, $R(|\mathbf{r}|)$ tends to zero. If periodic structures are present, $R(|\mathbf{r}|)$ will not tend to zero, but will have a periodic variation in $|\mathbf{r}|$ and the scale of segregation is defined by the correlation function

$$\xi = \int_0^\infty R(|\mathbf{r}|) d|\mathbf{r}|. \quad (14.16)$$

Another measure of goodness-of-mixing is the intensity of segregation, which indicates how sharp the compositional variations are. If diffusion is unimportant, the intensity of segregation is at a maximum, regardless of the spatial distribution of such compositional elements, and complete homogenization would produce a value of zero. For a two-component mixture of A and B it is defined as

$$I = \frac{\overline{C'_A{}^2}}{C'_A{}^2 C'_B{}^2}, \quad (14.17)$$

where I is the deviation of the concentrations in the segregated phases from the mean. These measures may be applied to the interpretation of outcrop scale systems. They provide a basis for comparison with forward models, and interpretation of scales of data, as statistical measures from, for example, crystal-scale features, may be assessed on the scales of meters to kilometers if outcrop is sufficiently extensive. The measures of spatial statistical significance are also present in the application of the variogram, a widely used element of geostatistics.

The potential energy for mixing may arise as a consequence of forcing by boundary conditions, or the decay of an unstable initial condition, or both; an example is mixing on reintrusion, which is likely to be important in geological systems (Jellinek & Kerr, 1999; Bergantz, 2000; Eichelberger *et al.*, 2000). Numerical experiments of transient, buoyant, multiphase cavity flow quantify the progress of mixing in terms of the Lyapunov exponent, σ_A (Williams, 1997), which is defined as

$$\sigma_A = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{dA(t)}{dA(0)}, \quad (14.18)$$

where $A(0)$ is the initial area and $A(t)$ is the area at a time after the start of stirring. A positive value of σ_A indicates an exponential increase of the surface area with time, and the reduction in the thickness of any region of distinct composition (the striation thickness). A kinematic description of the Lyapunov exponent is that it is the long-time average of the strain rate.

For a Reynolds number, Re , that is greater than $10^3 - 10^4$, turbulent stirring produces what is known as “Eulerian chaos.” This critical value of the Reynolds number is called the “mixing transition” (Breidenthal, 1981), and is associated with the notion of turbulence being fully developed where many scales of the flow are present. This critical value for the mixing transition is remarkably robust, being approximately the same for many different geometries and flow styles. The efficiency of stirring at high Re is the result of

straining and rapid exponential area increase in the smallest eddies of the turbulent flow. Mixing takes place by entrainment and nearly simultaneous dispersion. Hence, the rate-limiting aspects to the mixing are the time scales, usually the rotation period, of the largest eddies as they are the dynamic entities that dominate the entrainment (Brown & Roshko, 1974).

A salient point is that the striation thickness will decrease as

$$\frac{V}{A} \approx \eta e^{-\sigma_A t}; \quad \sigma_A \approx 0.3e_K, \quad (14.19)$$

where η is the characteristic length of the Kolmogorov microscale, and e_K the strain rate at this length scale. The Lyapunov exponent for these kinds of flows is always positive and the flow is formally chaotic. This is the kind of mixing that is most common in engineering and environmental flows and a thorough treatment is given by Baldyga and Bourne (1999). For a Re of 10^2 , the flow is in the convective regime, and the Lyapunov exponent is of 10^{-2} , indicating a flow that is transitional to chaotic. For a Re of 10^{-1} , the near absence of non-linear convective forces leads to a vanishing Lyapunov exponent, and the kinematics of mixing may change fundamentally.

Ultimately, the volume of perfectly mixed material is controlled by molecular diffusion. This diffusion process manifests the usual scaling and the volume, V , of mixed material after a time, t , is given by the proportionality

$$V \approx A\sqrt{Dt}, \quad (14.20)$$

where D is the diffusivity of the mixed component and A the surface area between mixing volumes. As D is a (non-constant) material property, the only way to increase the efficiency of mixing is to increase the surface area by stirring. This motivates the introduction of the striation thickness as one metric for the progress of mixing (Ottino, 1989), V/A . For volume-conserving incompressible materials, this is the scaled thickness of the unmixed volumes while stirring proceeds, and complete mixing is optimized in a system in which deformation reduces this length scale.

Viscosity contrasts are eventually rate-limiting for the efficiency of stirring, and these contrasts are determined by the thermal “lifetime” of the overall process. Thus, to be effective, the stirring must decrease the striation thickness of the pre-mixed volumes such that the thermal macro-scale of the process is equal to the time scale for compositional homogenization by diffusion

$$\frac{L^2}{(V/A)^2} \approx \frac{\kappa}{D}, \quad (14.21)$$

where L is the length scale associated with the overall thermal anomaly, and κ the thermal diffusivity. The ratio of the diffusivities will be of the order of from 10^4 to 10^8 depending on the definition of the components. For a diffusivity ratio of 10^6 and a thermal length scale of 1 km, the striation thickness must be reduced to 1 mm for molecular mixing to be achieved. This length scale may be smaller than the size of the crystals in multiphase flow, and illustrates the requirements and difficulty of complete mixing at the crystal scale.

Mixing of silicate melt and crystals may involve materials with differing viscosities and densities (Campbell & Turner, 1986; Sparks & Marshall, 1986; Jellinek & Kerr, 1999). The basic physics of mixing of variable property mixtures of magmas is complicated by the fact that temperature changes induce rheological changes through crystallization and exsolution of volatiles. None the less, it is instructive to consider some of the fundamentals of the variable property mixing of single-phase fluids (Burmester *et al.*, 1992; Rielly & Burmester, 1994; Jellinek & Kerr, 1999).

Consider, as a simple example, the intrusion of material into a magma accumulation site or chamber that is already in a state of unsteady motion. It has been shown that the efficiency of mixing depends on the ambient kinetic energy of the host mixture, the viscosity contrast, the density contrast, and the method of addition of the two materials. Mixing when high viscosity materials are added to a fluid environment in motion may only be effective if the inertial shear stresses associated with local unsteady motion may overcome the viscous stresses in the added material that resist stretching and entrainment. Thus, only the large eddies may distort the viscous additions leading to local break-up at large scales. It has been confirmed experimentally that the viscosity ratio is unimportant if

$$Re \frac{\mu_1}{\mu_2} \geq O(10^2), \quad (14.22)$$

where Re is the host environment Reynolds number, μ_1 the host viscosity, and μ_2 the viscosity of the addition. For values of this parameter group below this threshold, the mixing time may increase by orders of magnitude and the mixing will not be self-similar with respect to the Reynolds number.

The method of addition is also important, as that influences the surface area and hence the stresses. For example, material injected as a stream has a smaller characteristic length scale and will mix more readily than material added as clumps. The location of addition will influence the mixing as well unless the host is in a state of isotropic turbulence, which is unlikely in natural examples. Dense material added at the top in the form of a stream will be more likely to

mix than material added near the floor, as entrainment into down-going (multiphase?) plumes is likely.

Density differences also influence mixing – if added material is heavier, it has a tendency to sediment. This is a function of the Richardson number, Ri , which is proportional to the density contrast, or reduced gravity, between the added and resident materials. Assuming that the length scale in the Richardson number is that of the added material, and Ri is large, added material will sediment and tend to stay on the bottom, extending any delays in mixing associated with viscosity contrasts. Thus, effective mixing requires small density and viscosity contrasts, and addition at small length scales near the top of the system.

The “mixing” of immiscible fluids manifests two principle stages as a function of the capillary number, Ca , which is the ratio of the shear stress, τ , transmitted by the carrier phase and the resisting force, σ , associated with the drop interfacial tension and radius, R ,

$$Ca = \frac{\tau R}{\sigma}. \quad (14.23)$$

When Ca is greater than unity under conditions of equal viscosity, the mixing process is called “distributive mixing” and drops are extended affinely. As mixing proceeds, Ca tends to the critical value, disturbances grow, and break-up of the disperse phase occurs. This is called “dispersive mixing.” If the viscosity of the dispersed phase is less than the carrier phase, the micro-rheological processes and transition to dispersive mixing occur faster. The critical value of the capillary number for the transition between distributed and dispersive mixing is a function of the viscosity ratio and the flow kinematics, with the most effective dispersion not necessarily associated with a viscosity ratio of unity (Grace, 1982).

14.5 Heat transfer, melting, and rheological models

Changes in chemical potential are required for the production of a melt phase. These changes are usually the result of increasing temperature or the addition of volatiles or some combination of both. Estimating the role of fluid infiltration is hampered by the fact that it is often difficult to estimate the volatile content of newly added magmatic material into the crust, or to quantify the physical processes associated with volatile generation and transfer (cf., Holness & Clemens, 1999). Conversely, the consequences of heat transfer, often the rate-controlling step in crustal differentiation (Petford *et al.*, 1997; Harris *et al.*, 2000), are easier to estimate and predict.

We begin by noting that the discussion of heat transfer should first be developed explicitly in terms of enthalpy transfer, as the heat equation is based on the conservation of an extensive quantity, and secondly in terms of rates. It is incorrect to do a simple thermal balance, a popular but ad hoc calculation, which relates temperature changes between two bodies by simply equating their specific enthalpies and mass to an equilibrium temperature. In conjugate heat transfer (Bergantz, 1992), temperature changes are a function of the rates of heat transfer. The initial total enthalpy contrast may have no relation to the maximum temperatures experienced during the prograde step of a thermal event.

A simple example from conduction will suffice. Consider two semi-infinite regions in thermal contact. If these two regions were at constant temperature initially, the maximum temperature at their contact will be roughly the mean temperature regardless of how long the heat transfer takes place. Thus, the maximum temperature is not related to the actual amount of enthalpy exchanged. However, the integrated amount of heat transferred will depend on the initial specific enthalpy and the mass. So for a partial melting event, the amount of melt produced will depend on the magnitude of the enthalpy difference, but the maximum degree of melting will be determined only by the magnitude and spatial scale of the initial temperature contrast.

It is the interdependence between the phase relations and the temperature that determines the compositional spectrum of melts produced. In the simplest case, there is no melt transport during melting, and the phase relations and temperature equation (with initial and boundary conditions) provide a complete description of the system (Bergantz, 1990). It is important to appreciate that thermodynamic statements (e.g., the functional relationship between the enthalpy and temperature, or temperature and phase volume fraction) appear explicitly only as a prescribed closure condition. If the system is open, then one must have a complete description of the compositional phase space, as open system transport will change the progress of melting by changing the bulk composition of the system. One strategy for parameterization of the phase relation linked to a transport model is exemplified in Barboza and Bergantz (1997).

During a prograde thermal event, the maximum temperature dictates one of the compositional extremes and the maximum amount of melt. Melt composition and volume fraction dominate the rheology of the partially molten region and, hence, the transport styles and rates. There is an explicit feedback between rates of melting, maximum temperatures, and rheological states. This has been explored in detail for crustal melting associated with intrusion of mafic material into the crust (Barboza & Bergantz, 1996, 1997, 1998). These

studies indicate that the changes in rheological conditions associated with partial melting had a larger influence on the extent and progress of the melting than did changes in the phase diagram, or melt-fraction interval. Invoking assumptions that would optimize the conditions of enhanced heat transfer, these authors concluded that high degrees of melting, (e.g., greater than 40 vol.%) were not likely under most crustal conditions. This is in agreement with the estimated compositions of melts produced by natural protoliths, where greater amounts of partial melting produces melts that do not resemble natural examples (Beard & Lofgren, 1989).

Of course, if the mean temperatures of the host and intruding material produce melt fractions above this value (e.g., under conditions of a very steep geotherm) then even conduction would produce a mobile material above a critical melt fraction. However, it is notable that these conditions of rapid and extensive melting are rarely (ever?) reported in the rock record (Barton *et al.*, 1991). Hence, based on an overwhelming number of natural examples, as well as model analyses, magma once chambered, rarely produces thermal effects greater than that predicted assuming conductive heat transfer. The counter-examples, where magma has demonstrably been flowing in a dike or volcanic neck, often do melt the margins; see references in Knesel and Davidson (1999) and Davies and Tommasini (2000).

The rheological complexity of multiphase magmatic mixtures has been discussed by Vigneresse *et al.* (1996), Bagdassarov and Dorfman (1998), Vigneresse and Tikoff (1999) and Renner *et al.* (2000), and a comprehensive review of the rheology of suspensions may be found in Liu and Masliyah (1996). The notion that there is a single rheological critical melt fraction (RCMF) that limits melt transport is only applicable under nearly closed-system conditions, which may not occur often in natural samples (Sawyer, 1994). Rheological experiments do not reveal a single value for a RCMF (Rushmer, 1995; Rutter & Neumann, 1995; Bagdassarov & Dorfman, 1998) leaving it uncertain if there is a comprehensive constitutive model. In a compelling set of descriptive arguments combining outcrop-scale observations and experiments from material science, the notion of a RCMF has been extended by Vigneresse and Tikoff (1999) to include percolation thresholds to allow for phase-relative motion. While these distinctions lack a detailed theoretical description, they provide a very useful basis for developing more sophisticated models of multiphase mechanics at low to moderate local melt fraction.

However, one should be cautious about applying a comprehensive rheological model to multiphase systems subject to diverse kinematics (Iverson & Vallance, 2001). Buoyant flows involve both simple and pure shear; hence, constitutive equations must be developed for the entire range of flow

kinematics. In addition, rheological models of multiphase mixtures are implicitly dependent on the scale of averaging, or the scale of the stationary volume for the continuum. This sets the scales for any transport theory, whether formal or “back of the envelope;” this is discussed in more detail below.

A transport theory requires a statement of momentum balance, and if there is phase-relative motion, a momentum balance must be provided for each phase. Under these circumstances, the viscosity of the constituent phases of the mixture and multiphase drag interactions must be considered explicitly. The viscosity is then different in each transport equation and reverts to the literal definition, that it represents the drag of a phase on itself. Models for mixture viscosity that attempt to incorporate the physics of phase interaction by defining a “mixture” viscosity require a condition of no phase-relative motion. This means that there is only one local velocity for all phases. In our previous efforts in which a mixture rheological model was introduced (Barboza & Bergantz, 1997, 1998), we made it explicitly clear that there was no phase-relative motion, and this is a limitation of those works. Hence, the interpretation of the dynamics of outcrop-scale features manifesting prior melt-present conditions should be tempered with the notion that the invocation of a constitutive relationship requires an appreciation for the implicit assumption of length scales and possibility of phase-relative motion.

One consequence of partial melting is the development of porosity (Bergantz, 1990; Lupulescu & Watson, 1999) and the progressive development of melt transport networks (Brown, 1994; Sawyer, 2001). The interplay between the progress of melting, the development of a melt network, deformation, and melt migration, is complex (Brown & Solar, 1998a, 1998b; Marchildon & Brown, 2002, 2003; Guernina & Sawyer, 2003). Sawyer (2001) suggests that there are two end-member types of melt channel networks: (1) a melt-draining network that allows for within-layer melt redistribution, and (2) melt-transfer networks that allow melt to move across and out of its source layer. The melt-draining network moves melt from sites of incipient melting into a set of dynamic, hierarchical structures, the granularity of which is controlled by the foliation planes.

Rates of melt migration have been estimated based on the degree of chemical equilibration between leucosomes and protolith (Sawyer, 1991, 1994; Harris *et al.*, 2000). It has suggested that melt generation and deformation-assisted segregation may take place on the order of 10^2 years, although such rates have yet to be independently conformed based on an internally consistent physical model and consideration of a field study.

There is uncertainty as to the importance of the magnitude of the volume change and the appropriate form for the resulting permeability tensor for melt

migration, especially at water under-saturated conditions. Positive volume changes associated with muscovite dehydration melting may be around 2% (Patiño-Douce & Johnston, 1991; Connolly *et al.*, 1997; Rushmer & Brearley, 1998). This positive volume change may induce microfracturing, which may provide a means of generating permeability (Watt *et al.*, 2000), and Connolly *et al.* (1997) have estimated that the permeability may be 10^{-14} m² and isotropic. In contrast, Rushmer and Brearley (1998) caution that biotite dehydration may have small or negative volume changes, although Guernina and Sawyer (2003) document efficient melt removal, at up to 40% of melting, during regional biotite dehydration. Thus, it may be difficult to generalize the role of dehydration reactions in the production of porosity.

The cellular automaton approach provides one very promising, quasi-physical approach to exploring the means by which drainage networks develop (Miller & Nur, 2000). Although notable progress towards a master continuum models has been made (Connolly, 1997), a first-principles, comprehensive mechanical model for the progressive formation of kilometer-scale drainage networks that provides for melt to accumulate and migrate remains to be developed. It is often assumed that the Blake–Kozeny–Carman equation relating porosity to permeability is applicable. However, whether the permeability is anisotropic and what is the form of the tortuosity are both uncertain.

Recalling our discussion of granularity of data, there is always uncertainty as to whether regional suites of leucosomes were all present at the same time, and that their size reflects some measure of conditions at the time of putative melt transport. Two studies have considered natural examples, and one further study was motivated by metallurgical applications. In a novel study, Tanner (1999) concluded that the distribution of leucosomes was scale-invariant (fractal), allowing generalization to a simple transport model. He concluded that the melt could escape by buoyant flow alone, a conclusion that might warrant further consideration in light of a more complex transport model. Brown *et al.* (1999) conclude that melt channels were straight and uniform, suggesting that the flow may be regarded as a Darcy-like system on a regional basis. In an experimental study of the (dendritic) crystallization of metals, Nielsen *et al.* (1999) concluded that the Blake–Kozeny–Carman equation gave good agreement with experiments. The ability of melt to migrate during deformation also depends on the viscosity, which will vary as a function of melt composition as melting proceeds (Renner *et al.*, 2000).

In a study of pelite melting, Barboza and Bergantz (1996) considered the ratio of the permeability to the viscosity as a measure of likelihood of melt migration (Fig. 14.1.) and concluded that a melt fraction between 0.055 and 0.145 was more likely to be extracted than higher melt fractions. Although the

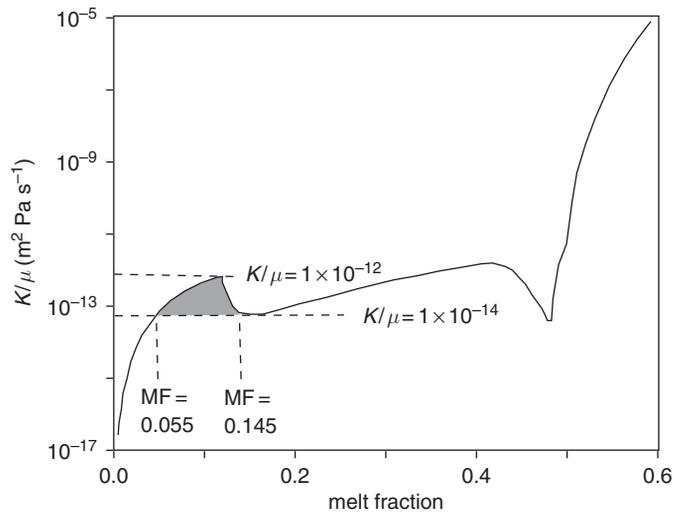


Fig. 14.1. Propensity for melt migration for pelite melting. The vertical axis is the ratio of the permeability divided by the melt viscosity. Higher values indicate a higher propensity for melt movement. Note that the values reached between melt fraction of 0.05 and 0.15 are not exceeded until after 40% of the pelite has been melted. Stippled region is the low melt fraction window of extractable melt.

permeability was not as high, the melt had a distinctly lower viscosity; hence, the ratio was greater. In summary, successful application of the methods used by Brown *et al.* (1999) and Tanner (1999), coupled with field observations (Sawyer, 1999, 2001; Marchildon & Brown, 2002, 2003) holds promise that more realistic models for permeability will emerge.

14.6 Transport models

Continuum macro-modeling may play an important role in illuminating aspects of the melt generation and transport, especially where the absence of real-time measurements makes direct verification difficult. We wish to distinguish our use of a continuum “macro-model” from, for example, a model for a mineral solution or a constitutive equation. Macro-models provide a means of isolating processes of interest, of exploring the behavior of systems characterized by extreme non-linearity, and at the very least are potent heuristic tools for developing intuition and insight. It is often said that one must start out with simple models to understand more complex systems. Of course, this cannot be literally true, as there is no guarantee that the super-position of the non-linear, perhaps simpler, processes will yield a system that resembles in any way a

combination of the added elements for coupled, non-linear systems. However, in our experience, working with simpler model systems is invaluable in that intuition is developed, experimental procedure refined, and confidence emerges. Additionally, models may provide significant insight into the construction of negative tests for a proposed process.

Models generally come in one of three classes (Kleinstreuer, 2003): analytical mathematical models, in which notions like a “semi-infinite strip” may be posited; experimental models, in which analog materials are arranged to explore kinematic states and process scaling; and, computer models, in which transport equations are discretized. Each of these models yields different information content at different scales of resolution as a function of their inherent observability. For example, the observability of an analog experiment might be related to the optics of the camera system, while the observability of the numerical experiment is dictated by the round-off error and the assumptions in the governing equations and discretization schemes (Roache, 1998). Thus, one must choose a model approach that represents some mixture of appropriate scale of observation, available resources and convenience.

In principle, one should be able to formulate a multiphase flow system in terms of the local and instantaneous variables. However, that necessitates recasting the system as a deforming multiboundary problem, and accounting for many of the micro-scale interactions, the forms of which may be unknown and that are rarely important at the macro scale. As a result, local averaging is used to define macro-scale variables, and some combination of the mixture or Eulerian or Lagrangian approaches is commonly used.

The mixture approach is an implicit multiphase model in which the field variables of all the phases are represented as being the same in any stationary volume. It is assumed that there is one “local” temperature for the multiphase mixture at every point, and that the local velocity is single-valued. Hence, if the system is in suspension flow, both the melt phase and the particle phases have the same velocity, or, if in the Darcy regime, the solid phases have zero velocity and the local velocity is the Darcy velocity of the melt phase (Oldenburg & Spera, 1992; Barboza & Bergantz, 1998). But regardless, there is only one local velocity. The advantages of the mixture approach are that the system dimensionality is reduced as there is virtually only one phase, with the construction of rather ad hoc constitutive equations to capture any multiphase interactions implicitly. It is also easier to use from the standpoint of algorithmic design, as standard techniques for single-phase flow computational fluid dynamics may be used. The disadvantages are the inability to model relative motion between phases, although at low Stokes’ number this is not a severe limitation. However, if one is interested in possible

relative motion in flow of a complex mixture like a diatexite, then the mixture approach may not be appropriate.

In the multiphase Eulerian approach, each of the phases is assumed to be a continuum, and the governing equations are assumed to hold at every point in the domain. This yields an elliptic system of equations in boundary value form. When averaged, information regarding the behavior of individual particles is lost, as the governing equations are cast in terms of the local volume fraction for each variable, which is identical to the existence probability of the phase occurring at that point. Assumptions are made regarding grain shape and size, and from the local volume fraction an interfacial area may be calculated. This is then used to calculate the drag and scalar transport. This approach is also called the “two-fluid” or Eulerian/Eulerian method, as it assumes that every phase is a virtual fluid even though one might be dealing with a particle–fluid mixture. This leads to some especially ad hoc constitutive relations, particularly in the scalar transport equations. For example, if one has a dispersed particle phase, what is the actual meaning of the within phase “thermal conductivity” if none of the elements of that phase are touching? There are a variety of constitutive functions to accommodate the interphase drag for the entire range of 0–100% liquid, with none seeming especially better than any other; hence, we recommend Agarwal and O’Neill (1988).

The Eulerian method is also subject to numerical diffusion, as discrete particles are represented by a field variable, the particle volume fraction. The numerical integration of field variables may lead to smearing of the interfaces as a consequence of numerical diffusion that occurs during numerical integration, and one must choose an advection scheme that aggressively reduces numerical diffusion (Andrews, 1995). However, the Eulerian method has been used widely in engineering design, and is the most commonly used multiphase theory in practice. It is reasonably robust when applied with awareness of its assumptions (Lahey & Bertodano, 1991). Further, elaboration of the nature of the Eulerian approach may be found in Durst *et al.* (1984) and Ni and Beckermann (1991), and geological examples in Bergantz and Ni (1999) and Valentine (1994).

Another approach for the physical description of a multiphase system would be to identify every occurrence of every phase, and follow their respective motions while accounting for all possible phase macro-interactions, phase change and properties. This is called the Lagrangian approach that yields a parabolic system and has the advantage of being straightforward, as the modeling of discrete particle interactions and heat transfer is mathematically simple. One distinct advantage is that particles may be tracked, and relative motion explicitly modeled. However, at the very least, the number of degrees of freedom

increases in direct proportion to the number of particles. For example, there would be about 10^7 crystals in a cubic meter of magma with 10 vol. % crystals, each with a diameter of 1 cm. And if the flow is fully turbulent, the number of degrees of freedom to describe the flow of the melt-phase varies as $Re^{9/4}$ where Re is the Reynolds number. Hence, for a Reynolds number of 10^5 , the melt phase alone requires the solution of 10^{11} linear equations. It is obvious that a strict Lagrangian approach is not feasible for turbulent or chaotic flow.

One refinement is to combine both Eulerian and Lagrangian methods. At moderate loadings of particles, the melt phase may be modeled as a Eulerian continuum, and the particles tracked individually as in the Lagrangian method. If the particle loadings are high, and the flow is coupled, one must employ iterative techniques involving cycling between the integration of the particle path and the state of the carrier phase as each depends on the other. Although this may slow down the calculations considerably, it is perhaps the most promising approach for the numerical investigation of diatexites. Sokolichin *et al.* (1997) have performed a comparison of the methods and the interested reader is directed there for further elaboration.

However, this approach is still not entirely satisfactory in that geological systems may be chaotic (i.e., small local changes may induce very different outcomes. Hence, any fully deterministic approaches like those described above will represent only one realization, and a strongly averaged one that is in effect a low-pass filter with regard to the spatial and temporal granularity of observations. One approach is the composite continuum–stochastic algorithm (Hersum & Bergantz, 2000) that will allow one to assess a range of possible outcomes or responses in a Monte Carlo sense. The new element of the algorithm is multigridding, in which hierarchical scales of gridding are used in space, time and methodology. By this we mean that a continuum, deterministic formulation of heat and mass transfer is developed in the usual way at averaging scales that are much larger than the grain scale. This reflects the controls that originate on the basic and usual transport constitutive laws. The finer scales, or sub-grids, are modeled using a stochastic approach to relate the distribution and transport of melt using either a cellular automaton approach or even simpler stochastic sweeping over a range of possible responses and outcomes. This approach allows one to assess the sensitivity to reasonable geological variability at a number of distinct scales and at each time step.

14.7 Closure

Crustal differentiation by melt generation and migration is a process with extreme granularity. The “memory” of these processes in the rock record is

both fractal and incomplete, with some events being over-represented. Rock memory is inevitably controlled by rheological transitions, which may vary at all scales and in highly local way throughout prograde-to-retrograde tectonic cycles. Rheological patchiness, representing in some combination local, but perhaps subtle, variations in protolith mode, state of hydration, and mineral fabric, controls the dynamics of melt transport and mixing, which are a consequence of the fundamentally multiphase character of crustal differentiation.

The absence of a comprehensive dynamic model for the interplay between the rate of change of chemical potential that induces melting, and the temporal and length scales of melt collection and transport, is the result of the local self organization that typifies multiphase dynamics. The transitions between end-member states such as heterogeneous porous flow, to transport of melt and residue in sheets and dikes, may be triggered by local stress focusing, reflecting non-general protolith conditions. The potentially rapid and local changes in the multiphase continuum may preclude the use of any approach based on field theories. Alternatively, a hierarchical approach, in which field theories are used to represent the energy and mass fluxes on average scales but are coupled to a stochastic or cellular automaton approach locally, may provide more insight in the range of possible kinematic responses and fluxes of energy and mass. The point is that, given the nature of observability between model approaches and natural examples, it does not seem likely that one will ever be able to test either a general modeling approach, or a particular geological case study with a detailed forward model.

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