

Melt ascent and differentiation from the upper mantle to the lower crust

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1 Introduction

In continental arc and rift volcanism erupting lavas are thought to be fed through trans-crustal magma processing systems extending down into the deep crust and mantle lithosphere. The magma source, however, is located even deeper down in the mantle asthenosphere, where decompression by upward mantle flow and/or fluxing by aqueous fluid infiltration lead to partial melting of hot mantle rock. The processes by which mantle melts first ascend into the base of the continental plate above and their rates and spatial distribution remain poorly understood. Current gaps in knowledge are due to, on one hand, the challenges in gaining sufficiently resolved data on these regions by geophysical imaging methods. The materials involved can only be sampled in few locations where lower crustal section have been tilted and eroded to reveal the roots of a transcrustal magmatic system, or through occasional xenoliths, rock pieces brought from depth to the surface in fast ascending magmas. On the other hand, modelling of melt ascent into the base of a plate is challenging due to a range of complex nonlinearities inherent in the problem. Mechanical interactions between melt and host rock are prone to instabilities and localisation feedbacks, leading to narrowly localised zones of enhanced melt flow and rock deformation. Thermochemical reactions between the phases can also lead to localising feedbacks such as dissolution channels solidification chimneys.

One possible way to gain better understanding of melt ascending into the deep crust is to use the chemistry of plutonic and volcanic igneous rocks as records of the dynamic process environments experienced during magma ascent and emplacement. This task is complicated by the fact that geochemical signatures in final rock products are the result of reaction and transport rates acting along a potentially protracted and circuitous trajectory through pressure-

23 temperature-composition space. Interpreting final compositions in terms of mass balancing
 24 models, whereby a composition is modelled as a mixture of assumed end-members (e.g., source
 25 rock, fractionated crystals, crustal assimilant), is widely practised but results are inherently
 26 non-unique.

27 In this contribution, we present a coupled thermo-chemical-mechanical model of melt ascent
 28 into the base of an overriding plate. The model includes two-phase mechanics including non-
 29 Newtonian rheology and decompaction failure, as well as a thermo-chemical model considering
 30 the evolution of melt fraction as a function of temperature and major-element composition, as
 31 well as tracking compactible and incompatible trace elements, and radiogenic and stable isotopic
 32 composition. The geochemical evolution model employs an idealised approach whereby the
 33 complex geochemistry involving a dozen major elements, a few minor elements and volatiles,
 34 tens of trace elements, and a diversity of radiogenic decay and stable isotope systems are
 35 reduced to few idealised components approximating some of the key behaviours of each aspect
 36 of geochemistry.

37 2 Method

38 2.1 Mechanical model

39 Melt ascent is modelled as the porous flow of an incompressible, viscous fluid through a per-
 40 meable and deformable matrix of incompressible, visco-plastic solid subject to decompaction
 41 failure. The non-dimensionalised governing equations expressing conservation of mass and mo-
 42 mentum in the two-phase mixture are,

$$43 \quad \nabla P = -\nabla p + \nabla \cdot \underline{\tau} + \phi B \hat{\mathbf{z}} , \quad (1a)$$

$$44 \quad \nabla \cdot \mathbf{V} = -\nabla \cdot \mathbf{v} , \quad (1b)$$

46 where $\mathbf{V} = [U, V, W]$ is the dynamic velocity, and P the dynamic pressure of the mixture,
 47 $\mathbf{v} = [u, v, w]$ the segregation velocity of the pore fluid, and p the compaction pressure and
 48 $\underline{\tau}$ the shear stress tensor of the solid matrix. $\nabla = [\partial/\partial x, \partial/\partial y, \partial/\partial z]$ is the partial spatial
 49 derivative. All variables and parameters are functions of position, $\mathbf{x} = [x, y, z]$, and time, t ,

50 unless indicated otherwise by a subscript nought. The unit vector of the depth coordinate,
 51 $\hat{\mathbf{z}}$, points in the direction of gravity. The dimensionless number B expresses the magnitude of
 52 buoyancy forces to tensile strength of the aggregate (more details below).

53 The dynamic velocity and pressure are each reduced by an invariant background field with
 54 constant spatial gradients. The dynamic pressure, P , is the Stokes pressure of the mixture
 55 reduced by a lithostatic background field, P_b , with $\nabla P_{\text{lith}} = [0, \rho_0 g_0]$, where ρ_0 is the constant
 56 solid matrix density, and g_0 the gravity constant. The dynamic velocity is the Stokes velocity of
 57 the mixture reduced by a background flow field, \mathbf{V}_b , which can assume both pure- and simple-
 58 shear flow patterns adjusted by dimensionless factors Pu, and Si which control the magnitude of
 59 shear stress induced by background deformation relative to the tensile strength of the aggregate.

60 The non-dimensionalised closures for segregation velocity, \mathbf{v} , compaction pressure, p , shear-
 61 stress tensor, $\underline{\boldsymbol{\tau}}$, and visco-plastic matrix rheology are,

$$62 \quad \mathbf{v} = -K (\nabla P + B\hat{\mathbf{z}}) , \quad (2a)$$

$$63 \quad p = -\frac{\eta}{\phi} \nabla \cdot \mathbf{V} , \quad (2b)$$

$$64 \quad \underline{\boldsymbol{\tau}} = \eta \dot{\underline{\boldsymbol{\epsilon}}} , \quad (2c)$$

$$65 \quad K = \left(\frac{\phi}{\phi_0} \right)^m \exp \left(-E^\ell \left[\frac{1}{T} - \frac{1}{T_0} \right] \right) , \quad (2d)$$

$$66 \quad \eta = \min \left(\exp \left(E^s \left[\frac{1}{T} - \frac{1}{T_0} \right] - \frac{\lambda}{F} (\phi - \phi_0) \right) \left(\frac{\dot{\epsilon}}{\dot{\epsilon}_b} \right)^{-n} , \frac{\tau_y}{\dot{\epsilon}} + \eta_{\min} \right) , \quad (2e)$$

$$67 \quad \tau_y = 1 + p . \quad (2f)$$

69 $\hat{\mathbf{z}}$ is the unit vector pointing along the depth coordinate. The shear strain rate tensor, $\dot{\underline{\boldsymbol{\epsilon}}}$, its
 70 components, and magnitude are defined as,

$$71 \quad \dot{\underline{\boldsymbol{\epsilon}}} = \frac{1}{2} (\nabla \mathbf{V} + \nabla \mathbf{V}^T) - \frac{1}{3} \nabla \cdot \mathbf{V} \underline{\mathbf{I}} , \quad (3a)$$

$$72 \quad \dot{\epsilon} = \sqrt{\frac{1}{2} \dot{\underline{\boldsymbol{\epsilon}}} : \dot{\underline{\boldsymbol{\epsilon}}}} . \quad (3b)$$

74 The rheological coefficients are centred on the reference melt fraction, ϕ_0 , temperature, T_0 ,
 75 and strain-rate $\dot{\epsilon}_b$. The matrix creep viscosity is weakened exponentially by the presence of
 76 melt with a factor $\lambda = 30$, by inverse temperature with the solid activation energy E^s , and

is softening as a powerlaw of the strain rate magnitude, $\dot{\epsilon}$, with a non-Newtonian powerlaw exponent $n = 2/3$. The reference strain-rate for the non-Newtonian powerlaw is determined by the applied pure- and/or simple-shear background deformation, $\dot{\epsilon}_b = |\text{Pu}| + |\text{Si}|$. Hence, the dimensionless shear viscosity, η , at $\phi = \phi_0$, $T = T_0$, and $\dot{\epsilon} = \dot{\epsilon}_b$ is equal to unity, and the compaction viscosity equal to ϕ^{-1} . Decompression failure is implemented using an effective-viscosity approach limiting shear stress as a function of compaction pressure so as not to exceed the tensile failure criterion, τ_y (see Fig. ??). A minimum yield viscosity, η_{\min} , is added to regularise the problem by imposing a minimum length scale of localised failure zones.

To highlight the role of decompression failure, we have scaled pressures and stresses by the tensile strength of the matrix, $p_o = \sigma_{T,0}$ to non-dimensionalise the problem. The dimensionless number $B = \Delta p_0 / \sigma_{T,0}$ expresses the relative magnitude of the buoyancy-related phase pressure difference, $\Delta p_0 = \Delta \rho_0 g_0 \delta_0$, relative to the tensile strength scale. The former is a natural scale of the Stokes-Darcy problem proportional to the matrix-melt density difference, $\Delta \rho_0$. Velocities are scaled by the Darcy speed scale $w_0 = K_0 p_0 / \ell_0$, and length by $\ell_0 = \sqrt{\eta_0 K_0}$, a natural scale of the problem related to the segregation-compaction length, $\delta_0 = \sqrt{\phi_0^{-1}} \ell_0$, where η_0 is the characteristic matrix shear viscosity, and $K_0 = a_0^2 \phi_0^m / (b_0 \mu_0)$ the Darcy coefficient scale, with a_0 the characteristic matrix grain size, $b_0 = 100$ a geometrical constant, and μ_0 the characteristic melt viscosity.

2.2 Thermo-chemical model

The thermo-chemical evolution by coupled reaction-transport processes in the partially molten mixture is modelled by a set of equations conserving energy, phase, and component mass, and

98 evolving trace and isotopic composition,

$$99 \quad \frac{\partial \phi}{\partial t} = \nabla \cdot (1 - \phi) \mathbf{v}^s + \Gamma, \quad (4a)$$

$$100 \quad \frac{\partial T}{\partial t} = -\bar{\mathbf{v}} \cdot \nabla T + \frac{\nabla^2 T}{\text{Pe}_T} - \frac{\Gamma}{\text{St}}, \quad (4b)$$

$$101 \quad \frac{\partial \bar{c}_{\text{maj}}}{\partial t} = -\nabla \cdot \bar{c}_{\text{maj}} \bar{\mathbf{v}} + \frac{\nabla^2 \bar{c}_{\text{maj}}}{\text{Pe}_c}, \quad (4c)$$

$$102 \quad \frac{\partial \bar{c}_{\text{tra}}}{\partial t} = -\nabla \cdot \bar{c}_{\text{tra}} \bar{\mathbf{v}} + \frac{\nabla^2 \bar{c}_{\text{tra}}}{\text{Pe}_c}, \quad (4d)$$

$$103 \quad \frac{\partial \bar{c}_{\text{irp}}}{\partial t} = -\nabla \cdot \bar{c}_{\text{irp}} \bar{\mathbf{v}} + \frac{\nabla^2 \bar{c}_{\text{irp}}}{\text{Pe}_c} - \Gamma_D, \quad (4e)$$

$$104 \quad \frac{\partial \bar{c}_{\text{ird}}}{\partial t} = -\nabla \cdot \bar{c}_{\text{ird}} \bar{\mathbf{v}} + \frac{\nabla^2 \bar{c}_{\text{ird}}}{\text{Pe}_c} + \Gamma_D, \quad (4f)$$

$$105 \quad \frac{\partial c_{\text{ist}}^s}{\partial t} = -\mathbf{v}^s \cdot \nabla c_{\text{ist}}^s + \frac{\nabla^2 c_{\text{ist}}^s}{\text{Pe}_c} - (c_{\text{ist}}^\Gamma - c_{\text{ist}}^s) \frac{\Gamma}{1 - \phi}, \quad (4g)$$

$$106 \quad \frac{\partial c_{\text{ist}}^\ell}{\partial t} = -\mathbf{v}^\ell \cdot \nabla c_{\text{ist}}^\ell + \frac{\nabla^2 c_{\text{ist}}^\ell}{\text{Pe}_c} + (c_{\text{ist}}^\Gamma - c_{\text{ist}}^\ell) \frac{\Gamma}{\phi}. \quad (4h)$$

108 The melt fraction, ϕ , evolves as a consequence of compaction, that is, divergence in the
 109 solid velocity field, \mathbf{v}_s , and (volumetric) melting rate, Γ . Sensible heat characterised by the
 110 temperature relative to the interval from lowest to highest melting point evolves as a function of
 111 advection by the mixture velocity field, $\bar{\mathbf{v}} = \phi \mathbf{v}^\ell + (1 - \phi) \mathbf{v}^s$, diffusion governed by the inverse of
 112 the thermal Peclet number, Pe_T , and sensible to latent heat conversion upon melting governed
 113 by the Stefan number, St . The major element composition of the mixture, $c_{\text{maj}} = \phi c_{\text{maj}}^\ell +$
 114 $(1 - \phi) c_{\text{maj}}^s$ evolves by divergence in the chemical flux, $c_{\text{maj}}^s \mathbf{v}^s + \phi c_{\text{maj}}^\ell \mathbf{v}^\ell$, and chemical diffusion
 115 governed by the chemical Peclet number, Pe_c . Note that chemical diffusivity of major elements
 116 is very slow on crustal length scale, hence chemical diffusion could be safely neglected in these
 117 models. We include it here for the purpose of regularisation to avoid growth of overly sharp
 118 compositional boundaries that can become numerically problematic for advection schemes. The
 119 phase compositions, $c_{\text{maj}}^{\ell,s}$ are functions of temperature and mixture composition defined by a
 120 phase diagram. Total mass conservation is observed by only solving for one phase, assuming
 121 that the mixture is saturated and both phase fractions sum to unity, and only solving for one
 122 major element component assuming that the two components also sum to unity (i.e., the lever
 123 rule applies).

124 The geochemical evolution of trace and isotopic compositions does not need to observe total

mass conservation since the elements involved are assumed to be present in trace quantities only. Hence, equations for all components are solved and no unity sum constraints apply. The mixture trace composition, c_{tra}^- follows the same form of conservation law as major element composition, with phase trace element compositions, $c_{\text{tra}}^{\ell,s}$, are set by partition coefficients, $K_{\text{tra}} = c_{\text{tra}}^s/c_{\text{tra}}^\ell$, here held constant for simplicity. Mixture concentrations of a set of parent and daughter isotopes linked by a radioactive decay system follow the same form of conservation law as major and trace components but are linked by the decay rate, $\Gamma_D = \bar{c}_{\text{irp}}/(\ln(2)D_{1/2})$, proportional to the concentration of the parent isotope, \bar{c}_{irp} , and the decay number, $D_{1/2}$, which is the dimensionless half-life. Stable isotopic composition of the melt and matrix phases are assumed to evolve only by advection on the phase velocity field and mass transfer between phases by phase-change reaction. Diffusion terms are added for the purpose of regularisation.

2.3 Numerical Implementation

The model is implemented in two dimension on a square domain of $L \times L$ non-dimensional size. The initial condition on temperature is a halfspace cooling solution representing a cool plate over a near-isothermal mantle. The initial major element concentration is a smoothed random noise to introduce some heterogeneity. The initial melt fraction is set to the equilibrium value given the temperature and bulk composition as specified by an idealised peritectic-eutectic phase diagram. The boundary conditions are free slip and insulating on the sides and free in/outflow and isothermal on the top and base. The side boundaries can be switched to periodic in models where horizontal simple shear dominates the background velocity.

The numerical implementation discretises the governing equations on a regular square grid of 500×500 finite-volume cells using a centred staggered-grid finite-difference scheme. Advection terms are implemented using flux-conservative centred or upwind-biased Fromm methods. The equations are solved using a damped Richardson iterative scheme. For reasons of numerical stability the shear visco-plasticity, η , and the phase reaction rate, Γ , are regularised by applying a small amount of Laplacian smoothing and lagged iteratively to avoid numerical oscillations. The mechanical part of the numerical algorithm was benchmarked against a manufactured analytical solution and shows second order error convergence with increasing spatial resolution. The simulation code was developed and tested in Matlab version R2020a and is openly available

¹⁵⁴ in on github.com/kellertobs/ivrea.