

General equations for modeling geochemical transport in open systems

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1 Introduction

This set of notes will try to set down in one coherent place, a general set of equations for calculating changes of major element, reactive trace element and U-series nuclides in an open system. Given the continuous form of the equations we will also deal with scaling and discrete forms using Semi-Lagrangian advection schemes.

The key to these derivations will be using general conservation of mass for a melt phase and a solid phase

$$\frac{\partial \rho_f \phi}{\partial t} + \nabla \cdot [\rho_f \phi \mathbf{v}] = \Gamma \quad (1)$$

$$\frac{\partial \rho_s (1 - \phi)}{\partial t} + \nabla \cdot [\rho_s (1 - \phi) \mathbf{V}] = -\Gamma \quad (2)$$

to rewrite the change in composition in the individual frames of the melt and solid. Here ρ_f, ρ_s are the densities of melt and solid, \mathbf{v}, \mathbf{V} are the melt and solid velocity fields, ϕ is the porosity and Γ is the total rate of mass transfer from solid to liquid ($\Gamma > 0$ is melting).

2 Major elements: fractional melting

In imposed fractional melting, a set of instantaneous melt compositions \mathbf{c}_{eq}^f are specified. These melts are locally in equilibrium with the solid residue and are assumed not to react with other liquids. With these compositions, conservation of composition for the melt and solid residue can be written

$$\frac{\partial \rho_f \phi \mathbf{c}^f}{\partial t} + \nabla \cdot [\rho_f \phi \mathbf{v} \mathbf{c}^f] = \mathbf{c}_{eq}^f \Gamma \quad (3)$$

$$\frac{\partial \rho_s(1-\phi)\mathbf{c}^s}{\partial t} + \nabla \cdot [\rho_s(1-\phi)\mathbf{V}\mathbf{c}^s] = -\mathbf{c}_{eq}^f \Gamma \quad (4)$$

where \mathbf{c}^f is the melt composition and \mathbf{c}^s is the solid composition. Note that all the concentrations are pseudo-vectors with N components that satisfy the closure rule $\sum_{i=1}^N c_i = 1$. With this requirement we can see that Eqs. (1) and (2) can be recovered directly from summing Eqs. (3) and (4) over all components. Nevertheless, it must also be true that for each element i , the RHS of these equations must be equal and opposite. This is a general feature of chemical conservation equations, that what leaves the solid must enter the liquid so that total mass is conserved. While these equations appear simple and have appropriate symmetries, it turns out to be more sensible to solve them numerically in a different form.

If we chain-rule the LHS of Eqs. (3)–(4) and substitute in (1)–(2) we can rewrite these equations as

$$\frac{D_f \mathbf{c}^f}{Dt} = (\mathbf{c}_{eq}^f - \mathbf{c}^f) \frac{\Gamma}{\rho_f \phi} \quad (5)$$

$$\frac{D_s \mathbf{c}^s}{Dt} = -(\mathbf{c}_{eq}^f - \mathbf{c}^s) \frac{\Gamma}{\rho_s(1-\phi)} \quad (6)$$

where

$$\frac{D_f}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \quad (7)$$

$$\frac{D_s}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla \quad (8)$$

are the material derivatives in the melt and solid frames respectively. Equation (5) states that the change in concentration experienced by the melt depends on the difference between the ambient melt composition and the instantaneous melt composition and is driven by the ratio of melt-production rate to the amount of available melt. In the limit that $\phi \rightarrow 0$ the melt composition goes to the instantaneous melt composition ($\mathbf{c}^f \rightarrow \mathbf{c}_{eq}^f$). Equation (6) is a similar equation for the solid composition but is integrated along solid flow lines.

2.1 Scaling

As always, it is useful to non-dimensionalize the equations a bit to make them consistent with all my other papers. For major elements, the concentrations are already dimensionless and of order 1 so there is no real need to scale them. However, we will scale ϕ , t and Γ in the usual way with

$$\phi = \phi_0 \phi' \quad (9)$$

$$t = \frac{\delta}{w_0} t' \quad (10)$$

$$\Gamma = \frac{\rho_s \phi_0 w_0}{\delta} \Gamma' \quad (11)$$

where ϕ_0 is a reference porosity, w_0 is the melt separation velocity at porosity ϕ_0 and δ is the compaction length defined at porosity ϕ_0 (see [1, 2] for details). Substituting into Eqs. (5)–(6) and dropping primes yields

$$\frac{D_f \mathbf{c}^f}{Dt} = \frac{\rho_s}{\rho_f} (\mathbf{c}_{eq}^f - \mathbf{c}^f) \frac{\Gamma}{\phi} \quad (12)$$

$$\frac{D_s \mathbf{c}^s}{Dt} = -\frac{\phi_0}{(1 - \phi_0 \phi)} (\mathbf{c}_{eq}^f - \mathbf{c}^s) \Gamma \quad (13)$$

2.2 Numerical Schemes

By writing these equations in terms of material derivatives, we can make extensive use of a very powerful numerical technique for advection schemes, the ‘‘Semi-Lagrangian’’ methods [3, 4] which combine the power of Lagrangian schemes based on the method of characteristics with Eulerian schemes that allow for solution on a regular grid. The actual integration scheme is more related to ODE techniques and requires finding the trajectory along which information will propagate to a given grid point and then doing high-order interpolation to evaluate line integrals along that trajectory. For example, the Semi-Lagrangian discretization for a problem with source terms

$$\frac{Dc}{Dt} = g(c, \mathbf{x}, t) \quad (14)$$

can be written using a Second order Runge-Kutta scheme as

$$\frac{c_{i,j}^{n+1} - c_{i',j'}^n}{\Delta t} = \frac{1}{2} [g_{i,j}^{n+1} + g_{i',j'}^n] \quad (15)$$

where $c_{i,j}^{n+1}$ is the unknown concentration at grid-location (i, j) and time-step $n + 1$ and $c_{i',j'}^n$ is the known concentration at time n but at the origin of the upwind trajectory that goes through point (i, j) . In general, this point is not on the grid and needs to be found using interpolation (I use bicubic interpolation in 2-D). Rearranging and using an alternative notation, we can write Eq. (15) as

$$c^+ = c^- + \frac{\Delta t}{2} [g^+ + g^-] \quad (16)$$

where $^+$ is understood to be at the grid point at time $n + 1$ and $^-$ is understood to be evaluated at the interpolated point at time n . Note, if there is no source term ($g = 0$) then the semi-Lagrangian scheme simply becomes $c^+ = c^-$ which is the expected solution from the method of characteristics. For melting problems, however, g is generally not zero and is usually a function of c resulting in either semi-implicit schemes or iterative schemes or both. The largest drawback to these

schemes is that they usually have to be hand-coded for each specific problem. Nevertheless, they have no Courant-condition, are a good representation of the underlying physics and are far superior to classical, simple advection schemes. Moreover, in open systems they allow you to track both melt and solid along separate trajectories but always react them on a regular grid. It's the only way to go really...and we will use these schemes extensively.

Anyway, for the case of fractional major element melting, we can write the discrete form of Eqs. (12)–(13) in the Semi-Lagrangian updating scheme as

$$\mathbf{c}^{f+} - \mathbf{c}^{f(f-)} = A^+(\mathbf{c}_{eq}^f - \mathbf{c}^f)^+ + A^{f-}(\mathbf{c}_{eq}^f - \mathbf{c}^f)^{f-} \quad (17)$$

$$\mathbf{c}^{s+} - \mathbf{c}^{s(s-)} = B^+(\mathbf{c}_{eq}^f - \mathbf{c}^s)^+ + B^{s-}(\mathbf{c}_{eq}^f - \mathbf{c}^f)^{s-} \quad (18)$$

where

$$A = \frac{\Delta t}{2} \left[\frac{\rho_s \Gamma}{\rho_f \phi} \right] \quad (19)$$

$$B = \frac{\Delta t}{2} \left[\frac{-\phi_0}{1 - \phi_0 \phi} \Gamma \right] \quad (20)$$

and f^- refers to the interpolated point along the melt trajectory and s^- is the interpolated point along the solid trajectory. All variables marked $^+$ occur at the same grid point at time $n + 1$. Rearranging for \mathbf{c}^{f+} and \mathbf{c}^{s+} yields the following update scheme

$$\mathbf{c}^{f+} = [(\mathbf{A}\mathbf{c}_{eq}^f)^+ + (\mathbf{A}\mathbf{c}_{eq}^f)^{f-} + (1 - A^{f-})(\mathbf{c}^f)^{f-}] / (1 + A^+) \quad (21)$$

$$\mathbf{c}^{s+} = [(\mathbf{B}\mathbf{c}_{eq}^f)^+ + (\mathbf{B}\mathbf{c}_{eq}^f)^{s-} + (1 - B^{s-})(\mathbf{c}^s)^{s-}] / (1 + B^+) \quad (22)$$

3 Reactive Trace elements: near fractional transport

A similar treatment can be worked out for simple trace elements undergoing fractional melting with the only addition that the instantaneous melt composition that is in equilibrium with the solid is simply $\mathbf{c}_{eq}^f = \mathbf{c}^s / \mathbf{D}$ where \mathbf{D} is a vector of bulk partition coefficients for each trace element.

In addition to fractional melting, however, it is also straightforward to add a reactive term to allow the tracer in the melt to try to re-equilibrate with the solid. Following the work on reactive melting of Aharonov et. al [5, 6] a simple approach to the reactive term is to use linear kinetics by adding a term for each element of form $R_i(c_i^s - D_i c_i^f)XS$, where R_i is the reaction rate for each element. A convenient assumption that allows these reactions to mimic diffusion between the solid and the liquid is to assume that $R_i \propto \rho_s \mathcal{D}_i^s / l^2$ where \mathcal{D}_i^s is the solid state diffusivity of component i and l is some nominal diffusional lengthscale (e.g. pore scale, channels

spacing etc. [7]). Thus it is possible to explore the behaviour of solid-liquid interaction without having to specify a particular microscopic model for solid-liquid diffusion although this is also a promising technique (e.g. see Iwamori [8, 9]). A comparison of the behaviour of the explicit diffusion and linear kinetics approaches is discussed by Bickle [10] for metamorphic problems.

With these assumptions, a general set of equations for evolution of trace element composition with reactive, near-fractional melting can be written

$$\frac{\partial \rho_f \phi \mathbf{c}^f}{\partial t} + \nabla \cdot [\rho_f \phi \mathbf{v} \mathbf{c}^f] = \frac{\mathbf{c}^s}{\mathbf{D}} \Gamma + \mathbf{R}(\mathbf{c}^s - \mathbf{D} \mathbf{c}^f) \quad (23)$$

$$\frac{\partial \rho_s (1 - \phi) \mathbf{c}^s}{\partial t} + \nabla \cdot [\rho_s (1 - \phi) \mathbf{V} \mathbf{c}^s] = -\frac{\mathbf{c}^s}{\mathbf{D}} \Gamma - \mathbf{R}(\mathbf{c}^s - \mathbf{D} \mathbf{c}^f) \quad (24)$$

The first term on the RHS of these equations is the addition (or subtraction) of an instantaneous fractional melt, the second term approximates the diffusion limited absorption of tracer by the solid when $\mathbf{c}^s < \mathbf{D} \mathbf{c}^f$ i.e. when the solid concentration is less than what would be in equilibrium with the ambient melt.

3.1 Scaling

Because melting models for trace elements only record changes from solid source compositions it is worth rescaling the equations. Physical scaling is given by Eqs. (9)–(11). For melt and solid it is useful to scale by the initial concentrations of each i.e.

$$\mathbf{c}^s = \mathbf{c}_0^s \mathbf{c}^{s'} \quad (25)$$

$$\mathbf{c}^f = \frac{\mathbf{c}_0^s}{\mathbf{D}_0} \mathbf{c}^{f'} \quad (26)$$

where \mathbf{c}_0^s and \mathbf{D}_0 are the solid source compositions and bulk partition coefficients for all elements at the initiation of melting.¹ Rewriting Eqs. (23)–(24) in terms of material derivatives, scaling and dropping primes yields the coupled sets of differential equations

$$\frac{D_f \mathbf{c}^f}{Dt} = \left(\frac{\mathbf{D}_0}{\mathbf{D}} \mathbf{c}^s - \mathbf{c}^f \right) \frac{\rho_s}{\rho_f \phi} [\Gamma + \mathbf{N}_{Da} \mathbf{D}] \quad (27)$$

$$\frac{D_s \mathbf{c}^s}{Dt} = -\mathbf{c}^s \left(\frac{1}{\mathbf{D}} - 1 \right) \frac{\phi_0 \Gamma}{1 - \phi_0 \phi} - \frac{\phi_0 \mathbf{N}_{Da}}{1 - \phi_0 \phi} \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right) \quad (28)$$

where

$$\mathbf{N}_{Da} = \frac{\mathbf{R} \delta}{\rho_s \phi_0 w_0} \quad (29)$$

¹Note: these equations do not assume that \mathbf{D} is constant.

is the vector of Damköhler numbers for each reaction defined as the amount of reaction experienced in the time it takes the melt flux to move a compaction length. For a diffusion controlled reaction the Damköhler number is very sensitive to the effective diffusivity and the diffusion length scale and can vary from anywhere from $0-10^4$ [7].

3.2 Numerical Schemes

Using the same semi-Lagrangian tricks as before, we can discretize Eqs. (27)–(28) with a second order Runge-Kutta scheme as before. If we define

$$A = \frac{\Delta t}{2} \left[\frac{\rho_s}{\rho_f \phi} [\Gamma + \mathbf{N}_{Da} \mathbf{D}] \right] \quad (30)$$

$$B = \frac{\Delta t}{2} \left[\left(\frac{1}{\mathbf{D}} - 1 \right) \frac{\phi_0 \Gamma}{1 - \phi_0 \phi} \right] \quad (31)$$

$$C = \frac{\Delta t}{2} \left[\frac{\phi_0 \mathbf{N}_{Da}}{1 - \phi_0 \phi} \right] \quad (32)$$

then the discrete form of Eqs. (27)–(28) becomes

$$\mathbf{c}^{f+} - \mathbf{c}^{f(f-)} = A^+ \left(\frac{\mathbf{D}_0}{\mathbf{D}} \mathbf{c}^s - \mathbf{c}^f \right)^+ + A^{(f-)} \left(\frac{\mathbf{D}_0}{\mathbf{D}} \mathbf{c}^s - \mathbf{c}^f \right)^{(f-)} \quad (33)$$

$$\mathbf{c}^{s+} - \mathbf{c}^{s(s-)} = -(B\mathbf{c}^s)^+ - (B\mathbf{c}^s)^{(s-)} - C^+ \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right)^+ - C^{(s-)} \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right)^{(s-)} \quad (34)$$

which is actually a coupled system of linear equations which can be written as

$$\begin{bmatrix} (1 + A) & -A\mathbf{D}_0/\mathbf{D} \\ -C\mathbf{D}/\mathbf{D}_0 & (1 + B + C) \end{bmatrix}^+ \begin{bmatrix} \mathbf{c}^f \\ \mathbf{c}^s \end{bmatrix}^+ = \mathbf{r} \quad (35)$$

$$\mathbf{r} = \begin{bmatrix} \mathbf{c}^{f(f-)} + A^{(f-)} \left(\frac{\mathbf{D}_0}{\mathbf{D}} \mathbf{c}^s - \mathbf{c}^f \right)^{(f-)} \\ (1 - B)^{(s-)} \mathbf{c}^{s(s-)} - C^{(s-)} \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right)^{(s-)} \end{bmatrix} \quad (36)$$

which is readily inverted for \mathbf{c}^{f+} and \mathbf{c}^{s+} given that the inverse of a 2×2 array is

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \quad (37)$$

and on the assumption that the matrix is not singular i.e. $\det \mathbf{A} = (1 + A)(1 + B) + C \neq 0$. Unfortunately, for large N_{Da} , the matrix actually is singular. This shouldn't be surprising because as the melt and solid move towards equilibrium,

there are no longer two distinct concentrations, I.e. if we know the melt concentration we know the solid and vice-versa. Simple tests on the above formulation suggest that the equations become stiff at relatively small values of N_{Da} and as $D \rightarrow 1$ (this needs to be checked). For this reason Eqs. (35)–(36) may only be good for near-fractional transport $N_{Da} \lesssim 1-10$ (?).

4 Reactive Trace elements: near equilibrium transport

For near-equilibrium transport, it may be more useful to rewrite Eqs. (23)–(24) in terms of the melt concentration \mathbf{c}^f and the *degree of disequilibrium*

$$\mathbf{u}^s = \mathbf{D}\mathbf{c}^f - \mathbf{c}^s \quad (38)$$

(this equation is unscaled) i.e. \mathbf{u}^s is the difference in concentration between the solid that would in equilibrium with the melt and the actual solid concentration. In equilibrium $\mathbf{u}^s = 0$. Alternatively we can think of the solid concentration $\mathbf{c}^s = \mathbf{D}\mathbf{c}^f - \mathbf{u}^s$ as the equilibrium solid concentration minus \mathbf{u}^s . To develop a set of equations for \mathbf{c}^f and \mathbf{u}^s it is first worth rewriting Eqs. (27)–(28) as

$$\frac{D_f \mathbf{c}^f}{Dt} = \mathbf{N}_{Da} \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right) \frac{\rho_s \mathbf{D}_0}{\rho_f \phi} \left[\frac{\Gamma}{\mathbf{N}_{Da} \mathbf{D}} + 1 \right] \quad (39)$$

$$\frac{D_s \mathbf{c}^s}{Dt} = \mathbf{c}^s \frac{(\mathbf{D} - 1) \phi_0 \Gamma}{\mathbf{D}(1 - \phi_0 \phi)} - \frac{\phi_0 \mathbf{N}_{Da}}{1 - \phi_0 \phi} \left(\mathbf{c}^s - \frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f \right) \quad (40)$$

4.1 Scaling

Equations (39)–(40) are dimensionless, to insert \mathbf{u}^s requires that we scale it as well. If we just assume that \mathbf{u}^s scales as \mathbf{c}_0^s then we end up with the indeterminate product $\mathbf{N}_{Da} \mathbf{u}^s$ as $\mathbf{N}_{Da} \rightarrow \infty$. A more sensible scaling is to assume

$$\mathbf{u}^s = \frac{\mathbf{c}_0^s}{\mathbf{N}_{Da}} \mathbf{u}^{s'} \quad (41)$$

and thus the dimensionless version of Eq. (38) is

$$\mathbf{u}^s = \mathbf{N}_{Da} \left(\frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f - \mathbf{c}^s \right) \quad (42)$$

and therefore Eqs. (39)–(40) can be written

$$\frac{D_f \mathbf{c}^f}{Dt} = -\mathbf{u}^s \frac{\rho_s \mathbf{D}_0}{\rho_f \phi} \left[\frac{\Gamma}{\mathbf{N}_{Da} \mathbf{D}} + 1 \right] \quad (43)$$

$$\frac{D_s}{Dt} \left[\frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f - \frac{\mathbf{u}^s}{\mathbf{N}_{Da}} \right] = -\mathbf{c}^f \frac{(1 - \mathbf{D}) \phi_0}{(1 - \phi_0 \phi) \mathbf{D}_0} \Gamma + \mathbf{u}^s \frac{\phi_0}{1 - \phi_0 \phi} \left[1 + \frac{(1 - \mathbf{D}) \Gamma}{\mathbf{N}_{Da} \mathbf{D}} \right] \quad (44)$$

4.2 Numerical Schemes

As before we can define

$$A = \frac{\Delta t}{2} \left[\frac{\rho_s \mathbf{D}_0}{\rho_f \phi} \left(\frac{\Gamma}{\mathbf{N}_{Da} \mathbf{D}} + 1 \right) \right] \quad (45)$$

$$B = \frac{\Delta t}{2} \left[\frac{(1 - \mathbf{D}) \phi_0}{(1 - \phi_0 \phi) \mathbf{D}_0} \Gamma \right] \quad (46)$$

$$C = \frac{\Delta t}{2} \left[\frac{\phi_0}{1 - \phi_0 \phi} \left(1 + \frac{(1 - \mathbf{D}) \Gamma}{\mathbf{N}_{Da} \mathbf{D}} \right) \right] \quad (47)$$

and write the discrete form of Eqs. (43)–(44) as

$$\mathbf{c}^{f+} - \mathbf{c}^{f(f-)} = -(\mathbf{A}\mathbf{u}^s)^+ - (\mathbf{A}\mathbf{u}^s)^{(f-)} \quad (48)$$

$$\left[\frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f - \frac{\mathbf{u}^s}{\mathbf{N}_{Da}} \right]^+ - \left[\frac{\mathbf{D}}{\mathbf{D}_0} \mathbf{c}^f - \frac{\mathbf{u}^s}{\mathbf{N}_{Da}} \right]^{(s-)} = -(\mathbf{B}\mathbf{c}^f)^+ - (\mathbf{B}\mathbf{c}^f)^{(s-)} + (\mathbf{C}\mathbf{u}^s)^+ + (\mathbf{C}\mathbf{u}^s)^{(s-)} \quad (49)$$

or rearranging for \mathbf{c}^{f+} and \mathbf{u}^{s+} we get

$$\begin{bmatrix} 1 & A \\ (\mathbf{D}/\mathbf{D}_0 + B) & -(C + 1/\mathbf{N}_{Da}) \end{bmatrix}^+ \begin{bmatrix} \mathbf{c}^f \\ \mathbf{u}^s \end{bmatrix}^+ = \mathbf{r} \quad (50)$$

$$\mathbf{r} = \begin{bmatrix} \mathbf{c}^{f(f-)} - (\mathbf{A}\mathbf{u}^s)^{(f-)} \\ (\mathbf{D}/\mathbf{D}_0 - B)^{(s-)} \mathbf{c}^{f(s-)} + (C - 1/\mathbf{N}_{Da})^{(s-)} \mathbf{u}^{s(s-)} \end{bmatrix} \quad (51)$$

which is invertible with

$$\det \mathbf{A} = - \left[C + \frac{1}{\mathbf{N}_{Da}} + A \left(\frac{\mathbf{D}}{\mathbf{D}_0} + B \right) \right]^+ \quad (52)$$

5 Uranium Series decay chains

Given a radioactive decay series $e_1 \rightarrow e_2 \rightarrow \dots e_n$ adding radioactive decay to reactive tracer codes is relatively straightforward. We begin by adding radioactive source and sink terms to Eqs. (23)–(24), which we now have to write in component form as

$$\frac{\partial \rho_f \phi c_i^f}{\partial t} + \nabla \cdot [\rho_f \phi \mathbf{v} c_i^f] = \frac{c_i^s}{D_i} \Gamma + R_i(c_i^s - D_i c_i^f) + \rho_f \phi [\lambda_{i-1} c_{i-1}^f - \lambda_i c_i^f] \quad (53)$$

$$\frac{\partial \rho_s (1 - \phi) c_i^s}{\partial t} + \nabla \cdot [\rho_s (1 - \phi) \mathbf{v} c_i^s] = -\frac{c_i^s}{D_i} \Gamma - R_i(c_i^s - D_i c_i^f) + \rho_s (1 - \phi) [\lambda_{i-1} c_{i-1}^s - \lambda_i c_i^s] \quad (54)$$

where λ_i is the radioactive decay constant for element i . Rearranging and scaling yields

$$\frac{D_f c_i^f}{Dt} = \left(\frac{D_{i0}}{D_i} c_i^s - c_i^f \right) \frac{\rho_s}{\rho_f \phi} [\Gamma + N_{Da}^i D_i] + \lambda_i \left[\frac{D_{0i}}{D_{0(i-1)}} c_{i-1}^f - c_i^f \right] \quad (55)$$

$$\frac{D_s c_i^s}{Dt} = -c_i^s \left(\frac{1}{D_i} - 1 \right) \frac{\phi_0 \Gamma}{1 - \phi_0 \phi} - \frac{\phi_0 N_{Da}^i}{1 - \phi_0 \phi} \left(c_i^s - \frac{D_i}{D_{i0}} c_i^f \right) + \lambda_i [c_{i-1}^s - c_i^s] \quad (56)$$

where here λ_i is dimensionless and equals $\lambda_i \delta / w_0$.² Note, this scaling assumes that the initial solid is in secular equilibrium, i.e.

$$\lambda_{i-1} c_{0(i-1)}^s = \lambda_i c_{0i}^s \quad (57)$$

5.1 Numerical Schemes

Defining a new constant

$$L_i = \frac{\Delta t \lambda_i}{2} \quad (58)$$

we can rewrite the discrete equations (35)–(36) as

$$\begin{bmatrix} (1 + A + L_i) & -AD_{i0}/D_i \\ -CD_i/D_{i0} & (1 + B + C + L_i) \end{bmatrix}^+ \begin{bmatrix} c_i^f \\ c_i^s \end{bmatrix}^+ = \mathbf{r} \quad (59)$$

$$\mathbf{r} = \begin{bmatrix} (1 - A - L_i)^{(f-)} c_i^{f(f-)} + (AD_{i0}/D_i)^{(f-)} c_i^{s(f-)} + L_i (D_{0i}/D_{0(i-1)}) (c_{i-1}^{f+} + c_{i-1}^{f(f-)}) \\ (1 - B - C - L_i)^{(s-)} c_i^{s(s-)} + (CD_i/D_{i0})^{(s-)} c_i^{f(s-)} + L_i (c_{i-1}^{s+} + c_{i-1}^{s(s-)}) \end{bmatrix} \quad (60)$$

Note that this system of equations is triangular. As long as $L_0 = 0$ we can solve, *at each point*, for the elements in sequence and the additional radioactive source term will always be available when needed. Pretty cool eh? Time to implement the bugger after I figure out how high a Damköhler number I can solve for in the near fractional limit. (so far $N_{Da} = 10$ is just peachy).

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²For passing to ridge calculations, it's probably more convenient to pass the dimensional decay rate, the depth of the melting region (or box) and the spreading rate. In this case $\lambda_i' = \lambda_i (d/U_0) (U_0'/z_{max})$ where U_0' and z_{max} are the dimensionless spreading rate and box depth in compaction lengths that are calculated within the program.

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