

HEAT3D: Magmatic Heat Flow Calculation

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The Heat3D code represents an evolving effort to quantify heat flow in and around magma bodies in order to better understand geothermal gradients in volcanic areas. As such the following documentation is also evolving. First the more analytical approaches are reviewed and their limitations in handling real-world effects of multiple dimensions, latent heat, and convection are mentioned. Then the numerical approach used in the Heat3D code is discussed. Heat3D also performs 2D calculations for problems where more approximate rapid results are desired. Users should keep in mind the potential affects of representing 3-D magma bodies in 2-D form, the general result being maximum cooling times being predicted. However, the code is capable of parallel computations, which are performed if the host computer has multiple processors or a hyperthreaded processor(s).

1. Analytical Approach

Analytical Theory. Assuming that the magma is emplaced instantaneously and that it experiences no further movement nor loss or gain of mass, the cooling and heat transfer is governed by conservation of energy:

$$\frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) - \mathbf{u} \cdot \nabla T + q , \quad (1)$$

where T is temperature, t is time, κ is thermal diffusivity, \mathbf{u} is the magma convective velocity vector, and q represents heat sources and sinks. This equation describes the change of temperature with time (left-hand-side; LHS) with the right-hand-side (RHS) summing the effects of thermal conductivity (first term), thermal convection (second term), heat sources and sinks (third term). For the following discussion of analytical approaches, I assume no convective heat transfer, which will be discussed in a later section. Secondly I assume that there are no heat sinks or source other than latent heat of magma crystallization.

To start the analysis, assume that there is no latent heat released during magma crystallization and no thermal property contrasts between the magma and host rock. First consider the case for 1-D cartesian coordinates, such that a magma body is represented by a slab of a finite thickness but of infinite length and width. These assumptions allow a 1-D expression of Eq. (1) as:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} , \quad (2)$$

for which x represents distance measured perpendicular to the surface of the slab. Analytical solution of Eq. (2) for geological systems has most commonly been achieved by assuming self-similarity of solutions (Carslaw and Jaeger, 1947) in which temperature is expressed non-dimensionally as θ .

$$\theta = \frac{T - T_0}{T_m - T_0}, \quad (3)$$

for which subscripts m and 0 refer to the initial temperature of the magma and host rock, respectively. A single similarity variable, η , can be defined that combines both temporal as spatial effects, and it is defined as the ratio of distance to twice the characteristic thermal diffusion distance:

$$\eta = \frac{x}{2\sqrt{\kappa t}}. \quad (4)$$

Rewriting Eq. (2) using non-dimensional temperature, θ , and the similarity variable, ξ , requires derivation of θ with respect to t and x in terms of η and reduces Eq. (2) from a partial differential equation to an ordinary differential equation:

$$-\eta \left[\frac{d\theta}{d\eta} \right] = \frac{1}{2} \frac{d^2\theta}{d\eta^2}. \quad (5)$$

In order to solve Eq. (5), one may define a variable $\varphi = d\theta/d\eta$ so that Eq. (5) becomes:

$$-\eta d\eta = \frac{1}{2} \frac{d\varphi}{\varphi}. \quad (6)$$

With Integration and exponentiation Eq. (6), one can show:

$$\frac{d\theta}{d\eta} = ce^{-\eta^2}, \quad (7)$$

in which c is a constant of integration. Considering the boundary between a magma and rock where $\eta = 0$, $\theta(0) \equiv 1/2$, integration of Eq. (7) yields:

$$\theta = c \int_0^\eta e^{-n^2} dn + 1/2, \quad \text{and} \quad \theta = c \int_{-\eta}^0 e^{-n^2} dn - 1/2, \quad (8)$$

for which n is an arbitrary integration variable. For the boundary condition $\theta(\infty) = 0$:

$$0 = c \int_0^\infty e^{-n^2} dn + 1/2; \quad \text{and for } \theta(-\infty) = 0: \quad 0 = c \int_{-\infty}^0 e^{-n^2} dn - 1/2. \quad (9)$$

For $n \geq 0$ the definite integral in Eq. (9) is equal to $\pi^{1/2}/2$, and the constant $c = -(2/\pi^{1/2})/2$ so that

$$\theta = 1/2 - \left(\frac{1}{2}\right) \frac{2}{\sqrt{\pi}} \int_0^{\eta} e^{-z^2} dz = 1/2 - \left(\frac{1}{2}\right) \text{erf}(\eta) = \left(\frac{1}{2}\right) \left[1 - \text{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right)\right], \quad (10a)$$

For $n \leq 0$, $c = (2/\pi^{1/2})/2$ and recalling that $\text{erf}(-\eta) = -\text{erf}(\eta)$ the solution is:

$$\theta = -1/2 + \left(\frac{1}{2}\right) \frac{2}{\sqrt{\pi}} \int_{-\eta}^0 e^{-z^2} dz = -1/2 - \left(\frac{1}{2}\right) \text{erf}(-\eta) = \left(\frac{1}{2}\right) \left[\text{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right) - 1\right]. \quad (10b)$$

Jaeger (1968) defines a problem for cooling of a sheet-like magma body of thickness, $2a$, intruded beneath deep cover, for which the x -axis origin is defined at the center of the sheet. For this problem θ must be evaluated away from both surfaces of the sheet ($x-a$ and $x+a$), and because the solution Eqs. (10a and 10b) are linear they can be summed:

$$\theta = \frac{1}{2} \left[1 - \text{erf}\left(\frac{x-a}{2\sqrt{\kappa t}}\right)\right] + \frac{1}{2} \left[\text{erf}\left(\frac{x+a}{2\sqrt{\kappa t}}\right) - 1\right] = \frac{1}{2} \left[\text{erf}\left(\frac{x+a}{2\sqrt{\kappa t}}\right) - \text{erf}\left(\frac{x-a}{2\sqrt{\kappa t}}\right)\right]. \quad (11)$$

Multiple Dimensions. The above equations are valid only in 1-D, which does not adequately model a cylindrical magma body of circular cross-section and a finite length. Consider the 3-D form of Eq. (2), expressed in cartesian coordinates:

$$\frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right). \quad (12)$$

Carslaw and Jaeger (1959) show the solution to Eq. (12) is similar to that of Eq. (11) but with added terms for the extra dimensions:

$$\theta = \left[\frac{1}{2} \left(\text{erf} \frac{x+a}{2\sqrt{\kappa t}} - \text{erf} \frac{x-a}{2\sqrt{\kappa t}} \right) \right] \left[\frac{1}{2} \left(\text{erf} \frac{y+b}{2\sqrt{\kappa t}} - \text{erf} \frac{y-b}{2\sqrt{\kappa t}} \right) \right] \left[\frac{1}{2} \left(\text{erf} \frac{z+c}{2\sqrt{\kappa t}} - \text{erf} \frac{z-c}{2\sqrt{\kappa t}} \right) \right], \quad (13)$$

for which a = the half-height, b = the half-width, c = the half-length of the magma body. Eq. (12) can be expressed using cylindrical coordinates with radial distance, r , azimuth ϕ , and length, z :

$$\frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \phi^2} + \frac{\partial^2 T}{\partial z^2} \right). \quad (14)$$

For magma bodies that approximate cylindrical shapes, use of cylindrical coordinates allows simplifying a 3-D problem to 2-D by assuming radial symmetry about the z -axis such that $\partial^2 T / \partial \phi^2 = 0$. Furthermore, if the heat source (magma body) can be represented by a cylinder whose length is much greater than its diameter (such as a conduit) then $\partial^2 T / \partial z^2$ vanishes for radial solutions midway along the cylinder at all times earlier than the z -coordinate diffusive time; this time can be easily determined for the value of the last term of Eq. (13), which is within 0.001% of unity for $\text{erf}(n)$ where $n \geq \pi$.

Letting $n \geq c/[2(\kappa t)^{1/2}] \geq \pi$, then $t \leq c^2/4\pi^2\kappa$. For example, a conduit of half-length $c = 500$ m and $\kappa = 0.0000004$ m²/s requires 500 years of cooling before the effects of the z axis begin to appear. With this consideration Eq. (14) is suitably expressed:

$$\frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial r^2} + \frac{\partial T}{r \partial r} \right). \quad (15)$$

From Carslaw and Jaeger [1959, §2.2(9)], the solution of Eq. (15) is that of an infinite cylinder where ω = the cylinder radius and from Carslaw and Jaeger's x -coordinate is replaced by r and their y -coordinate is set to zero ($z = 0$):

$$\theta = \frac{1}{2} \left(\operatorname{erf} \frac{r + \omega}{2\sqrt{\kappa t}} - \operatorname{erf} \frac{r - \omega}{2\sqrt{\kappa t}} \right) \left(\operatorname{erf} \frac{\omega}{2\sqrt{\kappa t}} \right) \quad (16)$$

Latent Heat and Thermal Property Contrasts. Addressing the issue of contrasting thermal properties between the magma and host rock, Delaney (1987) shows from work by Lovering (1936) the initial contact temperature as:

$$\theta_c = \frac{k_m / k_t}{k_m / k_t + \sqrt{\kappa_m / \kappa_t}}, \quad (17)$$

for which the subscripts m and t refer to the magma and host rock respectively. However, Delaney (1987) finds that although thermal property contrasts affect the maximum temperature achieved in the host rock, they do not have large influence over solutions at late times. In fact Delaney (1987) points out that most workers do not consider thermal property contrasts.

The effect of latent heat (L) production is not negligible, but as Delaney (1987) points out, there is no analytically exact method to include its effects. Assuming $L = 350$ kJ/kg, a first approximation of its effect is find an effective initial magma temperature, T_m^* , by adding to the temperature of the magma the amount L/c_m ($L/c_m = 350 \text{ kJ kg}^{-1}/1.2 \text{ kJ kg}^{-1} \text{ K}^{-1} = 292^\circ\text{C}$). Delaney (1987) finds that setting $T_m^* = T_m + L/c_m$ provides for adequate solutions for temperatures in host rocks at a distance of more than a quarter of a dike thickness away from the contact.

The main problem with the approximate approach for including the effect of latent heat is that temperature profiles within and near the magma body are not realistic and are too high. A more physically accurate method to account for latent heat is discussed by Turcotte and Schubert (1982); they follow the classical Stefan problem in which the cooling of a body of magma has a definite solidification temperature, $T_s = T_m$. Considering a 1-D case (slab-like geometry) and a magma intruded at $x < 0$, the solidification surface occurs at X_s :

$$X_s = -2\lambda\sqrt{\kappa t}, \quad (18)$$

for which λ is a constant to be determined. With this approach, one needs a solution that fits the conditions that $\theta = 1$ ($T = T_m = T_s$) where $x = X_s$. The solution implies that the temperature at any point, defined by η [from Eq. (4)] is proportional to the position of the solidification surface defined by λ :

$$\theta = \frac{\operatorname{erfc}(\eta)}{\operatorname{erfc}(-\lambda)} . \quad (19)$$

For $x \leq X_s$ $T = T_m$, and for $X_s < x < 0$, $T_m > T > T_i$. This solution is valid only for times at which latent heat is being released in the magma (i.e., the temperature at the hottest part of the magma, the center of the cody, is above the magma's solidus temperature).

Because $T_s = T_m$, solidification occurs immediately during cooling from T_m , releasing latent heat at a rate $\rho L(dx_m/dt)\delta t$, and by equating this rate with the rate of heat conduction by Fourier's law gives:

$$\rho L \left(\frac{dX_s}{dt} \right) = k \left(\frac{\partial T}{\partial x} \right)_{x=X_s} . \quad (20)$$

The derivative on the left-hand-side of Eq. (20) can be found by differentiating Eq. (18):

$$\frac{dX_s}{dt} = \frac{-\lambda\sqrt{\kappa}}{\sqrt{t}} . \quad (21)$$

The derivative on the right-hand-side of Eq. (20) can be found by differentiating Eq. (19):

$$\left(\frac{\partial T}{\partial x} \right)_{x=X_s} = \left(\frac{d\theta}{d\eta} \right)_{\eta=-\lambda} \left(\frac{\partial \eta}{\partial x} \right) (T_m - T_0) = \frac{-(T_m - T_0)}{2\sqrt{\kappa t}} \frac{2}{\sqrt{\pi}} \frac{e^{-\lambda^2}}{[1 + \operatorname{erf}(\lambda)]} \quad (22)$$

A transcendental equation of λ is given by substituting Eqs. (21) and (22) into Eq. (20) and recalling that $k = \rho c \kappa$:

$$\frac{L\sqrt{\pi}}{c(T_m - T_0)} = \frac{e^{-\lambda^2}}{\lambda[1 + \operatorname{erf}(\lambda)]} . \quad (23)$$

With Eqs. (19 and 23), temperatures in time and space can be calculated for 1-D problems that involve release of latent heat. Furthermore, Eq. (18) can be used to calculate the time for all the magma to solidify (i.e., when the solidification surface reaches the center of the slab and $X_s^2 = a^2$ where a is the slab half-thickness). The solidification time is a function of one-quarter of the area a^2 :

$$t_s = \frac{a^2}{4\kappa\lambda^2} \quad (24)$$

Considering cylindrical geometry, the area expressed by the term, a^2 , in Eq. (24) becomes $\pi a^2/4$. Replacing the cartesian position of the solidification surface by its cylindrical equivalent, R_s , Eq. (18) becomes:

$$R_s = -4\lambda\sqrt{\kappa t / \pi} , \quad (25)$$

and, the transcendental equation for λ is

$$\frac{4L / \pi}{c(T_m - T_0)} = \frac{e^{-\lambda^2}}{\lambda[1 + \operatorname{erf}(\lambda)]} \quad (26)$$

For given values of L , c , T_m , and T_0 , λ can be found by iteratively calculating the right-hand-side of Eq. (26) until it equals the left-hand-side. For a system where r is 0 at the contact between magma and host rock and increases towards the center of the magma body, the following solutions depend upon the value of R_s , which is a function of λ .

$$T = T_m \quad (r \geq R_s) \quad (27)$$

$$T = T_c \left(1 + \operatorname{erf} \frac{r}{2\sqrt{\kappa t}} \right) \left(\operatorname{erf} \frac{\omega}{2\sqrt{\kappa t}} \right) \quad (R_s > r) \quad (28)$$

where

$$T_c = T_0 + \frac{(T_s - T_0)}{1 + \operatorname{erf} \lambda} . \quad (29)$$

As Carslaw and Jaeger (1959) point out, there is no exact solution for a cylinder beyond its radius. Eq. (28) takes into account the cylindrical geometry in the same fashion as Eq. (16). As such, this solution is approximate, but comparisons of its calculated results with those from Eq. (16) show remarkable similarity, as will be discussed later. The solutions are valid for early-times when liquid magma (above its solidus) exists. The full solidification time occurs when the solidification surface, R_s , reaches the center of the magma heat source, and it is interesting to note that calculated maximum magma temperatures at this point in time can be very close to realistic solidus temperatures, even though they are not included in Eq. (26)

Because magma solidifies over a range of temperatures ($T_s < T_m$) and displays a small but finite contrast in thermal properties with host rock, one can follow the more complicated analysis of Carslaw and Jaeger (1959). For conditions where the conductivity of liquid and solid magma equal ($k_m = k_s$), the transcendental equation in λ from Carslaw and Jaeger (1959) can be modified for cylindrical geometry and property contrasts [cf. Carslaw and Jaeger (1959)]:

$$p \frac{\sqrt{\pi}(T_m - T_s)}{4T_s} = \frac{[1 - \operatorname{erf}(p\lambda)] \exp[(p^2 - 1)\lambda^2]}{\sigma + \operatorname{erf}(\lambda)} . \quad (30)$$

Eq. (30) account for the effects of latent heat by the variable p , which is the square-root of the ratio of diffusivities (κ) of the solid (subscript s) and liquid (subscript m). The magma diffusivity reflects the effect of a higher effective heat capacity from the addition of latent heat:

$$p = \left[\frac{\kappa_s}{k_m / \rho_m [c_m + L / (T_m - T_s)]} \right]^{1/2} . \quad (31)$$

The effect of property contrasts between the magma and host rock in Eq. (30) are accounted for by the variable, σ :

$$\sigma = \frac{k_m \sqrt{\kappa_r}}{k_r \sqrt{\kappa_m}} . \quad (32)$$

The solutions temperature are like those in Eqs. (27-29) and depend upon the temporal radial position of the cooling surface, R_s .

$$T_c = T_0 + \frac{\sigma(T_s - T_0)}{[\sigma + \operatorname{erf}(\lambda)]} \quad (33)$$

$$T = T_m \quad (r \geq R_s) \quad (34)$$

$$T = T_c \left(1 + \frac{1}{\sigma} \operatorname{erf} \frac{r}{2\sqrt{\kappa_m t}} \right) \left(\operatorname{erf} \frac{\omega}{2\sqrt{\kappa t}} \right) \quad (0 < r < R_s) \quad (35)$$

$$T = T_c \left(1 + \operatorname{erf} \frac{r}{2\sqrt{\kappa_t t}} \right) \left(\operatorname{erf} \frac{\omega}{2\sqrt{\kappa t}} \right) \quad (r < 0) . \quad (36)$$

Again the effect of cylindrical divergence is accounted for as in Eq. (28). Eqs. (30-36) take into account latent heat being released between T_m and T_s (solidus temperature) as well as property contrasts between the magma (subscript m) and host rock (subscript t). Compared to the calculation for latent heat where $T_s = T_m$, the effect of $T_s < T_m$ generally increases the length of time for complete solidification by ~20% (without property contrasts) to 200% (with property contrasts).

2. Numerical Approach

The Heat3D code solves heat flow by finite difference solution of energy and momentum conservation equations (i.e., Navier-Stokes) thereby getting around many of the problems and limitations of analytical approaches discussed above. These equations express heat transfer by conduction and convection with nonlinearities arising from variation of thermal conductivity in a non-

isotropic (heterogeneous) material and heat sources/sinks (e.g., latency). Natural convection involves not only convection within magmatic bodies but also within saturated permeable rock. The Boussinesq approximation and its importance in stating the Navier-Stokes equations is first presented in a general form. Then in geophysical applications, momentum conservation by Darcy's equation is employed because of its empirical success. Finally, discretization of the nonlinear partial differential equations involved is shown for the conductive, convective, and heat source terms of the energy conservation equation.

General. In the Boussinesq approximation, variations in ρ are ignored, except insofar as they give rise to a gravitational force. The continuity equation of fluid flow then becomes

$$\nabla \cdot (\rho \mathbf{u}) = \rho \nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{u} = 0 \quad . \quad (37)$$

The derivative term can also be rewritten

$$\rho \frac{D\mathbf{u}}{Dt} \approx \rho_0 \frac{D\mathbf{u}}{Dt} \quad . \quad (38)$$

The gravity force is

$$\mathbf{F} = \rho \mathbf{g} \quad , \quad (39)$$

where gravity is given by the gravitational potential

$$\mathbf{g} = -\nabla \phi \quad (40)$$

and

$$\rho = \rho_0 + \Delta\rho \quad (41)$$

The force due to gravity can then be rewritten

$$\begin{aligned} \mathbf{F} &= -(\rho_0 + \Delta\rho)\nabla\phi \approx -(\rho_0\nabla\phi + \phi\nabla\rho_0) - \Delta\rho\nabla\phi \\ &= -\nabla(\rho_0\phi) + \Delta\rho\mathbf{g} \end{aligned} \quad (42)$$

since

$$\nabla\rho_0 \approx 0 \quad . \quad (43)$$

Now, let

$$P' \equiv P + \rho_0\phi \quad . \quad (44)$$

The Navier-Stokes equations are the fundamental partial differential equations that describe the flow of incompressible fluids. Using the rate of stress and rate of strain tensors, it can be shown that the components F_j of a viscous force \mathbf{F} in a nonrotating frame are given by momentum conservation

$$\frac{F_i}{V} = \frac{\partial}{\partial x_j} \left[\eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \nabla \cdot \mathbf{u} \right] \quad (45)$$

where η is the dynamic viscosity, λ is the bulk viscosity, also called the second viscosity coefficient (Tritton 1989), $\nabla \cdot \mathbf{u}$ is the divergence, and Einstein summation has been used to sum over $j = 1, 2,$ and 3 . Now, for an incompressible fluid, the divergence $\nabla \cdot \mathbf{u} = 0$, so the λ term drops out.

F_i consists of F_v (viscous force), F_p (pressure force), and F_b (body force), where

$$\frac{F_v}{V} = \eta \nabla^2 \mathbf{u}, \quad \frac{F_p}{V} = -\nabla p, \quad \text{and} \quad \frac{F_b}{V} = \Delta \rho \mathbf{g}$$

The Navier-Stokes equation for flow then becomes

$$\rho_0 \frac{D\mathbf{u}}{Dt} = -\nabla p + \eta \nabla^2 \mathbf{u} + \Delta \rho \mathbf{g} \quad (46)$$

Linearize $\Delta \rho$ with temperature using the thermal expansion coefficient α

$$\Delta \rho = -\alpha \rho_0 \Delta T \quad (47)$$

And divide by ρ_0 , remembering that kinematic viscosity is $\nu = \eta/\rho$ to obtain momentum conservation:

$$\frac{Du}{Dt} = -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 u - g \alpha \Delta T \quad (48)$$

With the addition of an equation for temperature, this will complete the Boussinesq equations. Let \mathbf{H} be the conductive heat flux and J be the heat generated per unit volume.

$$\mathbf{H} = -k \nabla T \quad (49)$$

Energy conservation is expressed as

$$\rho c_p \frac{DT}{Dt} = -\nabla \cdot \mathbf{H} + J \quad (50)$$

where c_p is the constant pressure heat capacity such that with division by ρc_p we get

$$\frac{DT}{Dt} = \nabla \cdot \left(\frac{k}{\rho c_p} \nabla T \right) + \frac{J}{\rho c_p} \quad (51)$$

Equations (37)-(51) are the Boussinesq convection equations. The terms in these equations are given the following names where $-g\Delta T$ is the buoyancy force, $k\nabla^2 T$ is the heat conduction term, $J/(\rho c_p)$ is the heat generation term, and $\mathbf{u} \cdot \nabla T$ is the advection term. If the buoyancy force is the sole cause of motion, the convection is termed free convection. If the buoyancy force is negligible, the convection is termed forced convection.

Expanding the full derivatives, defining the thermal diffusivity $\kappa \equiv k/\rho C_p$, and setting $q = J/\rho C_p$ the Boussinesq convection equations are for momentum and continuity

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\rho_0} \nabla p - \mathbf{u} \cdot \nabla \mathbf{u} + \nu \nabla^2 \mathbf{u} - g\alpha \Delta T \quad (52)$$

and for energy conservation

$$\frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) - \mathbf{u} \cdot \nabla T + q \quad (53)$$

Geophysical Application. Conductive and convective energy transfer are specified in Eq. (53), and for water-saturated porous rock, \mathbf{u} can be calculated while conserving momentum with the Darcy equation:

$$\mathbf{u} = -\frac{\mu}{\eta} (\nabla p - \mathbf{F}_b) \quad (54)$$

where μ is the permeability, η is the fluid dynamic viscosity (viscous forces), ∇p is the fluid pressure gradient (buoyancy), and F_b is the hydrostatic (body) force. Now let's consider the balance of the buoyant force and body force inside the brackets of Eq. (54). For the hydrostatic case pressure acts downward:

$$\mathbf{F}_b = \rho_0 \mathbf{g} \quad (55)$$

The fluid pressure gradient is related to a change in density with temperature [Eqs. (42) and (47)] by:

$$\nabla p = \rho \mathbf{g} = (\rho_0 + \Delta \rho) \mathbf{g} = (\rho_0 - \rho_0 \alpha \Delta T) \mathbf{g} \quad (56)$$

so that for upward convection to occur, the buoyant force must exceed the body force

$$\left(\frac{\partial p}{\partial z} - \rho \mathbf{g} \right) = [\rho_0 - (\rho_0 - \rho_0 \alpha \Delta T)] \mathbf{g} = \rho_0 \alpha \Delta T \mathbf{g} \quad (57)$$

Then Eq. (54) becomes

$$\mathbf{u} = \frac{\mu}{\eta} (\rho_0 \alpha \Delta T \mathbf{g}) \quad (58)$$

So permeability and thermal conductivity are important factors in determining heat flow in porous media, but the conductivity is affected by the presence of fluid saturated pores such that an effective conductivity k_e must be considered:

$$k_e = nk_w + (1 - n)k_r \quad (59)$$

where subscripts w and r refer to water and rock, respectively, and n is the porosity. Also thermal conductivity varies with temperature and pressure, and the following relationship from Chapman and Furlong (1991) expresses that variation:

$$k(T, z) = k_0 \left(\frac{1 + cz}{1 + bT} \right) \quad (60)$$

Where convection will occur can be determined by the value of the system's thermal Rayleigh number, a ratio of buoyant and viscous forces:

$$Ra = \frac{g \alpha H^3 \Delta T}{\eta k} \quad (61)$$

where H is the height of the fluid system. In general where $Ra > 1000$ to 2000 convection will occur. For a fully saturated aquifer where the system length scale is determined by a network of pores, permeability is an important limitation, Ra may be expressed as:

$$Ra = \frac{\rho g \alpha \mu H \Delta T}{\eta k_e} \quad (62)$$

convection will set in where

$$\frac{\partial T}{\partial z} > \frac{4\pi^2 \kappa^2 \eta}{k_e \rho g \alpha H^2} \quad \text{or where } Ra > 4\pi^2 \quad (63)$$

For magmas convection can be represented as occurring in a vertical pipe driven by the pressure gradient, and Eq. (58) can be replaced by the Poiseuille equation for viscous flow:

$$\mathbf{u} = \frac{r^2}{8\eta L} (\rho_0 \alpha \Delta T \mathbf{g}) ; \quad (64)$$

in which r is the effective pipe radius and L is the distance over which a fluid pressure gradient exists. Magmas below their liquidus temperature are multiphase materials dominated by the liquid and crystals, the former of which is lighter than the latter. During convection because of density contrasts, Stokes flow exists and the liquid moves past the crystals to some degree, resulting in crystal settling. This phenomena is strongly temperature dependent such that during cooling as the solidus temperature is approached, the fraction of liquid present decreases and the network of inter-crystal passage ways becomes more restrictive, adding a kind of permeability effect. Thus one can view liquid convection in magma impeded by crystals; thus, the value of $r^2/(8L)$ in Eq. (64) can be replaced by a temperature-dependent expression of liquid permeability as a function of solid-fraction porosity.

Method for Numerical Solution of Conductive Heat Flow. Starting with the differential equation for heat conduction only, which is of parabolic form:

$$\frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) \quad (65)$$

expand derivatives in 3-D Cartesian coordinates:

$$\frac{\partial T}{\partial t} = \frac{\partial \kappa_x}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial \kappa_y}{\partial y} \frac{\partial T}{\partial y} + \frac{\partial \kappa_z}{\partial z} \frac{\partial T}{\partial z} + \kappa_x \frac{\partial^2 T}{\partial x^2} + \kappa_y \frac{\partial^2 T}{\partial y^2} + \kappa_z \frac{\partial^2 T}{\partial z^2} , \quad (66)$$

or alternatively in 3-D cylindrical coordinates:

$$\frac{\partial T}{\partial t} = \frac{\partial \kappa_r}{\partial r} \frac{\partial T}{\partial r} + \frac{1}{r} \frac{\partial \kappa_\theta}{\partial \theta} \frac{1}{r} \frac{\partial T}{\partial \theta} + \frac{\partial \kappa_z}{\partial z} \frac{\partial T}{\partial z} + \kappa_r \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) + \kappa_\theta \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \kappa_z \frac{\partial^2 T}{\partial z^2} . \quad (66a)$$

Heat3D uses 3-D Cartesian coordinates. An explicit forward time-centered space (FTCS) scheme is the simplest numerical approach, is a first-order approximation, and is inherently stable (Crank, 1956); however, an explicit Dufort-Frankel scheme is a second-order approximation and unconditionally stable, and an implicit Crank-Nicholson scheme is also unconditionally stable and should provide a somewhat faster solutions. For this study, I demonstrate the FTCS and Dufort-Frankel methods.

The finite difference solution requires discretization of derivatives following general rules (e.g., Differentiated Stirling approximation); for example for fictitious quantity A:

$$dA/dx = \Delta A/\Delta x = [A(j+1) - A(j-1)] / 2\Delta x . \quad (67)$$

and

$$\begin{aligned} dA^2/dx^2 &= \Delta (\Delta A/\Delta x) / \Delta x &= \{ [A(j+1) - A(j)] / 2x \} - [A(j) - A(j-1)] / 2x \} / x \\ & &= [A(j+1) - 2 A(j) + A(j-1)] / \Delta x^2 . \end{aligned} \quad (68)$$

For simplicity, I use the following notation:

$$\begin{aligned}
T^n &= \text{forward time temperature} & T^o &= \text{backward time temperature} \\
\kappa_x &= \kappa_x(i, j) & \kappa_{x1} &= \kappa_x(i, j-1) & \kappa_{x2} &= \kappa_x(i, j+1) \\
T &= T(i, j) & T_{x1} &= T_x(i, j-1) & T_{x2} &= T_x(i, j+1) \\
\kappa_y &= \kappa_y(i, j) & \kappa_{y1} &= \kappa_y(i-1, j) & \kappa_{y2} &= \kappa_y(i+1, j) \\
T_{y1} &= T_y(i-1, j) & T_{y2} &= T_y(i+1, j)
\end{aligned} \tag{69}$$

Using cell-averaged values for coefficients of derivatives:

$$\begin{aligned}
A(j-1) &= [A(j-1) + A(j)]/2 & A(j+1) &= [A(j+1) + A(j)]/2 \\
A(j) &= [A(j-1) + A(j+1)]/2 = [A(j-1) + 2A(j) + A(j+1)]/4
\end{aligned} \tag{70}$$

$$\begin{aligned}
(T^n - T) / [\Delta t] &= [(\kappa_{x2} - \kappa_{x1}) / (2\Delta x)] [(T_{x2} - T_{x1}) / (2\Delta x)] \\
&+ [(\kappa_{y2} - \kappa_{y1}) / (2\Delta y)] [(T_{y2} - T_{y1}) / (2\Delta y)] \\
&+ [(\kappa_{z2} - \kappa_{z1}) / (2\Delta z)] [(T_{z2} - T_{z1}) / (2\Delta z)] \\
&+ [T_{x1}(\kappa_{x1} + \kappa_x)/2 - 2T_x(\kappa_{x1} + 2\kappa_x + \kappa_{x2})/4 + T_{x2}(\kappa_x + \kappa_{x2})/2] / (\Delta x^2) \\
&+ [T_{y1}(\kappa_{y1} + \kappa_y)/2 - 2T_y(\kappa_{y1} + 2\kappa_y + \kappa_{y2})/4 + T_{y2}(\kappa_y + \kappa_{y2})/2] / (\Delta x^2) \\
&+ [T_{z1}(\kappa_{z1} + \kappa_z)/2 - 2T_z(\kappa_{z1} + 2\kappa_z + \kappa_{z2})/4 + T_{z2}(\kappa_z + \kappa_{z2})/2] / (\Delta x^2)
\end{aligned} \tag{71}$$

For $\Delta x = \Delta y = \Delta z$

$$\begin{aligned}
T^n - T &= [\Delta t / (\Delta x^2)] [(\kappa_{x2}T_{x2} - \kappa_{x2}T_{x1} - \kappa_{x1}T_{x2} + \kappa_{x1}T_{x1})/4] \\
&+ [\Delta t / (\Delta x^2)] [(\kappa_{y2}T_{y2} - \kappa_{y2}T_{y1} - \kappa_{y1}T_{y2} + \kappa_{y1}T_{y1})/4] \\
&+ [\Delta t / (\Delta x^2)] [(\kappa_{z2}T_{z2} - \kappa_{z2}T_{z1} - \kappa_{z1}T_{z2} + \kappa_{z1}T_{z1})/4] \\
&+ [\Delta t / (\Delta x^2)] [(\kappa_{x1}T_{x1} + \kappa_xT_{x1})/2 - 2(\kappa_{x1}T_x + 2\kappa_xT_x + \kappa_{x2}T_x)/4 + (\kappa_xT_{x2} + \kappa_{x2}T_{x2})/2] \\
&+ [\Delta t / (\Delta x^2)] [(\kappa_{y1}T_{y1} + \kappa_yT_{y1})/2 - 2(\kappa_{y1}T_y + 2\kappa_yT_y + \kappa_{y2}T_y)/4 + (\kappa_yT_{y2} + \kappa_{y2}T_{y2})/2] \\
&+ [\Delta t / (\Delta x^2)] [(\kappa_{z1}T_{z1} + \kappa_zT_{z1})/2 - 2(\kappa_{z1}T_z + 2\kappa_zT_z + \kappa_{z2}T_z)/4 + (\kappa_zT_{z2} + \kappa_{z2}T_{z2})/2]
\end{aligned} \tag{72}$$

$$\begin{aligned}
T^n = T &+ [\Delta t / (\Delta x^2)] \\
&\{ [D_{x1}T_{x1} - 2D_xT_x + D_{x2}T_{x2}] + [D_{y1}T_{y1} - 2D_yT_y + D_{y2}T_{y2}] + [D_{z1}T_{z1} - 2D_zT_z + D_{z2}T_{z2}] \}
\end{aligned} \tag{73}$$

where:

$$\begin{aligned}
D_{x1} &= (3\kappa_{x1} + 2\kappa_x - \kappa_{x2}) / 4 ; & D_{x2} &= (3\kappa_{x2} + 2\kappa_x - \kappa_{x1}) / 4 & D_x &= (\kappa_{x1} + 2\kappa_x + \kappa_{x2}) / 4 ; \\
D_{y1} &= (3\kappa_{y1} + 2\kappa_y - \kappa_{y2}) / 4 ; & D_{y2} &= (3\kappa_{y2} + 2\kappa_y - \kappa_{y1}) / 4 & D_y &= (\kappa_{y1} + 2\kappa_y + \kappa_{y2}) / 4 ; \\
D_{z1} &= (3\kappa_{z1} + 2\kappa_z - \kappa_{z2}) / 4 ; & D_{z2} &= (3\kappa_{z2} + 2\kappa_z - \kappa_{z1}) / 4 & D_z &= (\kappa_{z1} + 2\kappa_z + \kappa_{z2}) / 4 ;
\end{aligned}$$

Although stability of the numerical solution of Eq. (73) is guaranteed by the Courant-Friedrich-Lewy (CFL) stability condition ($\Delta t < 0.5 \Delta x / D_{max}$), it is important to note with the above formulation that some values of D can be negative, which reflects a dominating effect of the diffusivity gradient and can cause numerical instability. This problem is corrected by using more conservative values of D :

$$\begin{aligned}
D_{x1} &= (\kappa_{x1} + \kappa_x) / 2 ; & D_{x2} &= (\kappa_{x2} + \kappa_x) / 2 & D_x &= (\kappa_{x1} + 2\kappa_x + \kappa_{x2}) / 4 ; \\
D_{y1} &= (\kappa_{y1} + \kappa_y) / 2 ; & D_{y2} &= (\kappa_{y2} + \kappa_y) / 2 & D_y &= (\kappa_{y1} + 2\kappa_y + \kappa_{y2}) / 4 ; \\
D_{z1} &= (\kappa_{z1} + \kappa_z) / 2 ; & D_{z2} &= (\kappa_{z2} + \kappa_z) / 2 & D_z &= (\kappa_{z1} + 2\kappa_z + \kappa_{z2}) / 4 ;
\end{aligned}$$

The Dufort-Frankel scheme solves the temporal derivative $(T^n - T^o)/2\Delta t$ by replacing $(2DT)$ terms in Eq. (73) by $(DT^n + DT^o)$. Defining

$$a \equiv 2(D_x + D_y + D_z)\Delta t / 3\Delta x^2, \quad (74)$$

one can express this scheme, retaining the anisotropy (heterogeneity) of diffusivities:

$$T^n = \left(\frac{1-3a}{1+3a} \right) (T^o) + \left(\frac{2\Delta t / \Delta x^2}{1+3a} \right) [D_{x1}T_{x1} + D_{x2}T_{x2} + D_{y1}T_{y1} + D_{y2}T_{y2} + D_{z1}T_{z1} + D_{z2}T_{z2}]. \quad (75)$$

Method for Solution of Convective Heat Flow. The differential equation is shown below:

$$\frac{\partial T}{\partial t} = -\mathbf{u} \cdot \nabla T = -\frac{K}{\eta} (\rho_0 g \alpha \Delta T) \cdot \nabla T \quad (76)$$

In Eq. (74) K represent parameters appropriate for either Darcy (Eq. 58) or Poiseuille (Eq. 64) flow. Numerical solutions of Eq. (74) are very sensitive to temperature gradients and prone to be unstable, unless explicit mass and momentum conservation are simultaneously satisfied. Alternatively by observing limiting boundary conditions, solutions to Eq. (76) can approximate the effects of convection in a fashion that numerically mimics effective diffusivity.

$$T^n = T + [\Delta t / \Delta 2x] [\mathbf{u}_x (T_{x1} - T_{x2}) + \mathbf{u}_y (T_{y1} - T_{y2}) + \mathbf{u}_z (T_{z1} - T_{z2})], \quad (77)$$

For which the velocity vectors \mathbf{u}_x , \mathbf{u}_y , and \mathbf{u}_z are found through Eqs. (58 and 64) and stability is insured by the CFL stability used in Eq. (73).

Method for Solution of Heat Sources/Sinks. By assuming an explicit temperature range over which crystallization/melting occurs, a constant latent heat of fusion/crystallization, and a linear relationship between crystal content and temperature over this range, an iterative solution is possible. For Heat calculations this simplification is represented by:

$$\frac{\partial T}{\partial t} = -\frac{Q_l \delta T}{(c_p + 1) \Delta T_{sl}} = \frac{Q_l}{(c_p + 1) \Delta T_{sl}} (T - T^n); \quad (78)$$

for which heat is expressed in kJ, Q_l is the latent heat, c_p is heat capacity, δT is an incremental change in temperature by conduction and convection ($T^n - T$ from Eqs. 36 and 38), and ΔT_{sl} is the temperature difference between the liquidus and solidus. For $Q_l = 350$ kJ/kg, $c_p = 1$ kJ/kg-K, and $\Delta T_{sl} = 350$ K, Eq. (76) states that for $\delta T =$ two degrees of cooling by conduction/convection there is one degree heat added by crystallization. For these values, iterative solution of Eq. (78) results in addition of 350 kJ/kg of heat to the magma for cooling from the liquidus temperature to the solidus.

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