

A numerical study of nucleation, growth and settling of crystals from a turbulent convecting fluid

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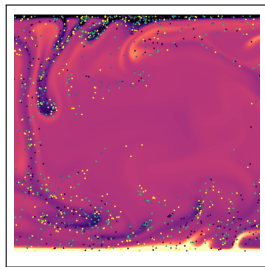
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Cooling magma is of interest to geologists, petrologists, as well as planetary physicists. Solidified magma chambers are exposed for direct observation in several places on Earth, but the freezing of magma within these bodies is not. Existing numerical models typically parametrize the nucleation, growth, and sedimentation of solid crystals in such systems. Here we present preliminary results from direct numerical simulations of these processes.



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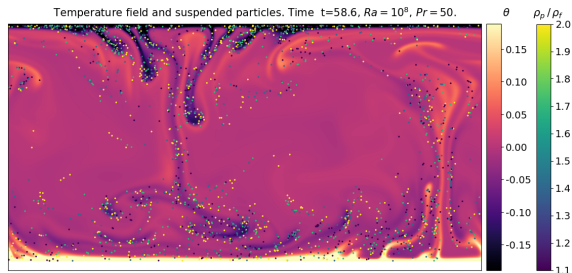


Abstract

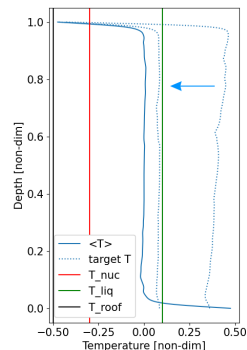
To our knowledge, a direct numerical model of crystal generation, growth, dynamics, and sedimentation in a cooling magmatic body is non-existent. In this study we make the first steps toward constructing such model. We evaluate the equilibrium concentration of a thermally convecting suspension that is cooled from above and in which solid crystals are self-consistently generated in the thermal boundary layer near the top. In a previous study (Patočka et al., 2020), we investigated the settling rate of solid particles suspended in a highly vigorous ($Ra = 10^8, 10^{10}$, and 10^{12}), finite Prandtl number ($Pr = 10, 50$) convection. In this follow-up study we additionally employ the model of crystal generation and growth of Jarvis and Woods (1994), instead of using particles with a predefined size and density that are uniformly injected into the carrier fluid.

We perform a series of numerical experiments of particle-laden thermal convection in 2D and 3D Cartesian geometry using the freely available code CH4 (Calzavarini, 2019). Starting from a purely liquid phase, the solid fraction gradually grows until an equilibrium is reached in which the generation of the solid phase balances the loss of crystals due to sedimentation at the bottom of the fluid. For a range of predefined density contrasts of the solid phase with respect to the density of the fluid ($\rho_p/\rho_f = [0, 2]$), we measure the time it takes to reach such equilibrium. Both this time and the equilibrium concentration depend on the average settling rate of the particles and are thus non-trivial to compute for particle types that interact with coherent structures of the turbulent convecting flow (see Patočka et al., 2020).

In this preliminary study we consider the fluid to be in statistically steady state of basally heated Rayleigh-Bénard convection. In our target applications, a hot magma will be enclosed in a fixed temperature cavity (blue dashed lines in figure on the right). If the time to reach equilibrium crystal distribution is much smaller than the overall cooling of the chamber, then the evolutionary target simulation should behave as a sequence of statistically steady states. We investigated four types of particle types defined via their density contrast, $\rho_p / \rho_f = 1.1, 1.4, 1.7, 2.0$ (color of the dots).



Particles are nucleated only for temperatures below T_{nuc} and grow in size if $T < T_{\text{liq}}$. In [Res: TBL](#) only the TBL is below the liquidus (first stage of cooling), while in [Res: bulk](#) the situation is depicted by the solid lines below ($\bar{T} < T_{\text{liq}}$).



Fluid dynamics

In terms of non-dimensional quantities, the Navier-Stokes equations read:

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \sqrt{\frac{Pr}{Ra}} \nabla^2 \mathbf{u} + \theta \hat{\mathbf{z}} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\partial_\tau \theta + (\mathbf{u} \cdot \nabla) \theta = \frac{1}{\sqrt{PrRa}} \nabla^2 \theta, \quad (3)$$

where $\mathbf{u}$ is the fluid velocity and θ is the fluid temperature. Ra and Pr are the Rayleigh and Prandtl number that control the flow characteristics:

$$Ra := \frac{\alpha g \Delta T H^3}{\nu \kappa}, \quad Pr := \frac{\nu}{\kappa}. \quad (4)$$

Initial and boundary conditions

In this study we consider well developed convection states as the initial condition. Top and bottom boundaries are at constant temperature, corresponding to basally heated Rayleigh-Bénard convection. Side-walls are periodic. Presumably, a cooling magma in nature can be described as a sequence of equilibrium states (Jarvis and Woods, 1994). See [Setup](#) for a visual representation and discussion.

Particle dynamics

In terms of non-dimensional quantities, the simplified Maxey-Riley equation for computing particle trajectories reads:

$$\frac{dv}{dt} = \beta \frac{Du}{Dt} + \frac{1}{St}(u - v) + \Lambda \hat{z}, \quad (5)$$

with u being the fluid and v the particle velocities. The three non-dimensional control parameters are:

$$\beta = \frac{3\rho_f}{\rho_f + 2\rho_p}; \quad St = \frac{r_c^2 \sqrt{\alpha g \Delta T}}{3\nu\beta\sqrt{H}}; \quad \Lambda = \frac{\beta - 1}{\alpha \Delta T}. \quad (6)$$

The Stokes number St is the particle response time τ_D divided by the characteristic time H/u^* , where H is magma chamber height. It describes the viscous friction acting on each particle due to the difference between particle and fluid velocity. The parameter Λ (hereafter buoyancy ratio) expresses the relative importance of particle buoyancy with respect to the thermally-induced buoyancy of the fluid (the unit vector $\hat{z}$ points vertically upward).

Units

To scale the non-dimensional time to **physical time**, we use the term “terminal distance”, t.d.= $St \Lambda t = V_{\text{Stokes}} t_{\text{physical}}/H$, i.e. it is the distance a given particle would travel within time t in a non-convecting fluid, divided by the size of the magma chamber. On the left figure in [Res: bulk](#) we provide terminal distance for selected crystal types (their size taken as the average from the obtained size distributions).

To scale the non-dimensional particle radius to **physical length**, one must not only multiply the value by the characteristic size H , but also by $(Ra_{\text{ref}}/Ra)^{0.25}$ in order to account for the inflated crystal size resulting from the impossibility to numerically model the target Rayleigh number Ra_{ref} (Patočka et al., 2020). This affects also the obtained solid fraction plotted in [Res: SF](#) – we, in fact, predict dilute equilibrium suspensions.

Particle nucleation and growth (kinetic laws)

Growth rate of crystals is given by (eqs 3.9, 5.1, 5.4, and 5.6 in Jarvis and Woods (1994)):

$$V(\Delta T) = \frac{dr_p}{dt} = V_{\text{ref}} \times \left(\frac{T_L(h, \Phi) - T_p}{\Delta T_{\text{ref}}} \right)^q, \quad (7)$$

where T_L is the depth (h) and composition (solid fraction Φ) dependent liquidus, T_p is the particle temperature, T_{top} is the roof temperature that is chosen to represent the reference temperature. The denominator is the reference temperature drop ΔT_{ref} (labeled as ΔT in the notation of Jarvis and Woods (1994) – see their Eq. 5.1). The dummy variable of V is $\Delta T := T_L(h, \Phi) - T_p$ and denotes the undercooling in the position of a crystal (undercooling of the isothermal convective bulk in Jarvis and Woods (1994))

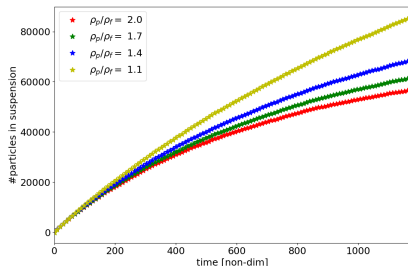
The number of nucleated crystals per unit volume is given by (eqs 3.8, 5.1, 5.4, and 5.6 in Jarvis and Woods (1994)):

$$\tilde{N}(\Delta T) = \tilde{N}_{\text{ref}} \left(\frac{T_L(h, \Phi) - T - E}{\Delta T_{\text{ref}} - E} \right)^p. \quad (8)$$

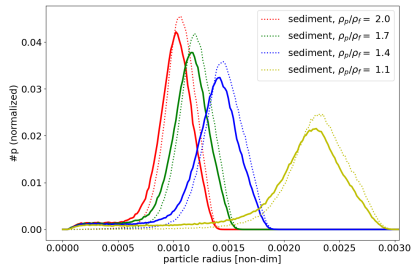
Note that I use $\Delta T := T_L(h, \Phi) - T$ as the dummy variable of $\tilde{N}$, while Jarvis and Woods (1994) quite crudely assume that the entire “nucleating” boundary layer is at the roof temperature T_{top} and they use $T_L(h, \Phi) - T_{\text{top}}$ as the independent variable of $\tilde{N}$ (see their eq. 3.8). $\tilde{N}_{\text{ref}}$ is the reference nucleation rate $\tilde{N}(\Delta T_{\text{ref}})$, to be discussed later

The prefactors V_{ref} and N_{ref} are poorly constrained. One of the aims of this study is to constrain these by comparing obtained particle size distributions with observations.

Before the entire bulk of the fluid cools below the liquidus, it is only the thermal boundary layer that can host crystal nucleation and growth. First we thus investigate the scenario in which only the TBL is below the liquidus. Re-melting is not considered in the figures below. The cooling system must go through this “TBL growth” stage before solids start to grow within the whole model domain.

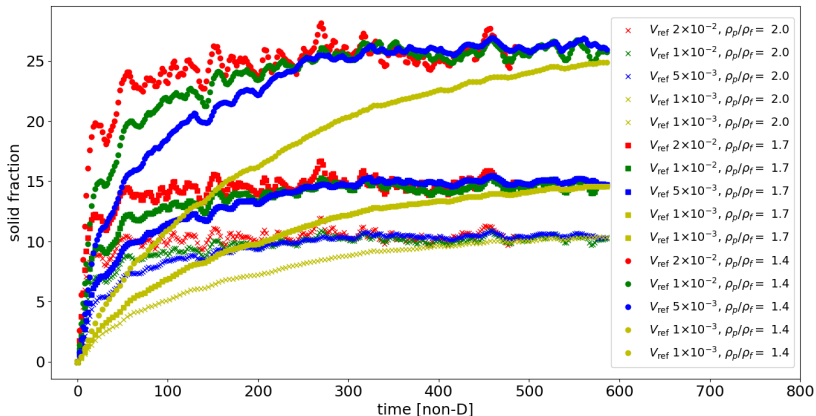


After some time, equilibrium is reached between crystal nucleation and sedimentation and the number of particles in suspension becomes constant. For TBL growth this time is larger than for bulk growth (cf. [Res: bulk](#)). In both cases the time can be order of magnitude larger than the terminal time (see [Eqs: trajectories](#)).

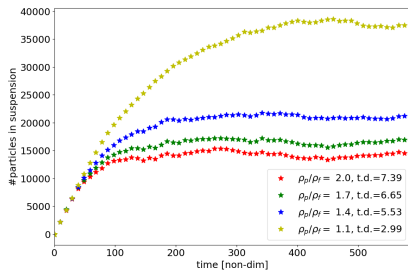


The resulting particle size distribution is gaussian-like for each particle type. Note that there is no abundance of near-zero sized particles - since these are observed in nature, they must be nucleating within the sedimentary layer itself. For converting the particle sizes to real units, see [Eqs: trajectories](#). Solid lines represent suspension, dashed are for sediment.

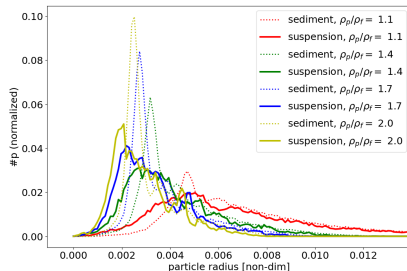
One of the interesting results from the first stage of magma chamber cooling, the TBL growth stage, is that the obtained solid fraction (i.e. concentration field) does not depend on the growth rate prefactor V_{ref} . This is because with larger V_{ref} spend less time in suspension, which compensates for their increased size (solid fraction = #particles $\times$ average particle volume / fluid volume)



As soon as the bulk of the fluid cools below the liquidus, nucleated crystals can grow within the entire model domain and thus reach larger sizes.



While the time to reach equilibrium is shorter here than in [Res: TBL](#), it is still a multiple of the terminal time, i.e. the time each particle type would take to sink through the chamber if magma was not convecting (marked by t.d. in the figure legend, for physical units see [Eqs: trajectories](#)).



Particle size distribution in suspension (solid lines) and sediment (dashed) for the statistically stationary situation depicted in [Setup](#). While tails of the obtained distributions resemble those observed in nature, the lack of near-zero sized particles indicate that these must nucleate outside the top TBL.

- ▶ The laws for nucleation and growth of solid crystals are poorly constrained for most mineral types under the pressure and temperature conditions that are expected in natural magma chambers. Here we construct a numerical model of cooling magma with the aim to constrain these laws by comparing the obtained equilibrium size distribution of crystals in sediment with observations.
- ▶ The time to reach equilibrium may be substantially longer than the characteristic Stokes sinking time of the crystals. This may be important for the application of the quasi-steady assumption of Jarvis and Woods (1994). In other words, cooling must be slow in order to view evolution of the system as a series of stationary situations.
- ▶ We study two stages of the cooling process. In the first one, only the thermal boundary layer is cold enough for the crystals to grow. In the second stage, the entire fluid bulk is below the liquidus, allowing for crystal growth at all depths. We show that both these stages may leave their record in the sediment.
- ▶ The obtained size distribution of sedimented crystals lacks abundance of near-zero sized particles, contrary to natural observations. This indicates that particle nucleation must be important also within the forming sedimentary layer itself, and not only near the chamber roof.

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