Mathematical Models for Simultaneous Particle Dissolution and Nucleation during Heat Treatment of Commercial Aluminium Alloys

Jos de Zwaan

Numerical Analysis Group
Department of Applied Mathematics
Delft University of Technology

November 30, 2005

Outline

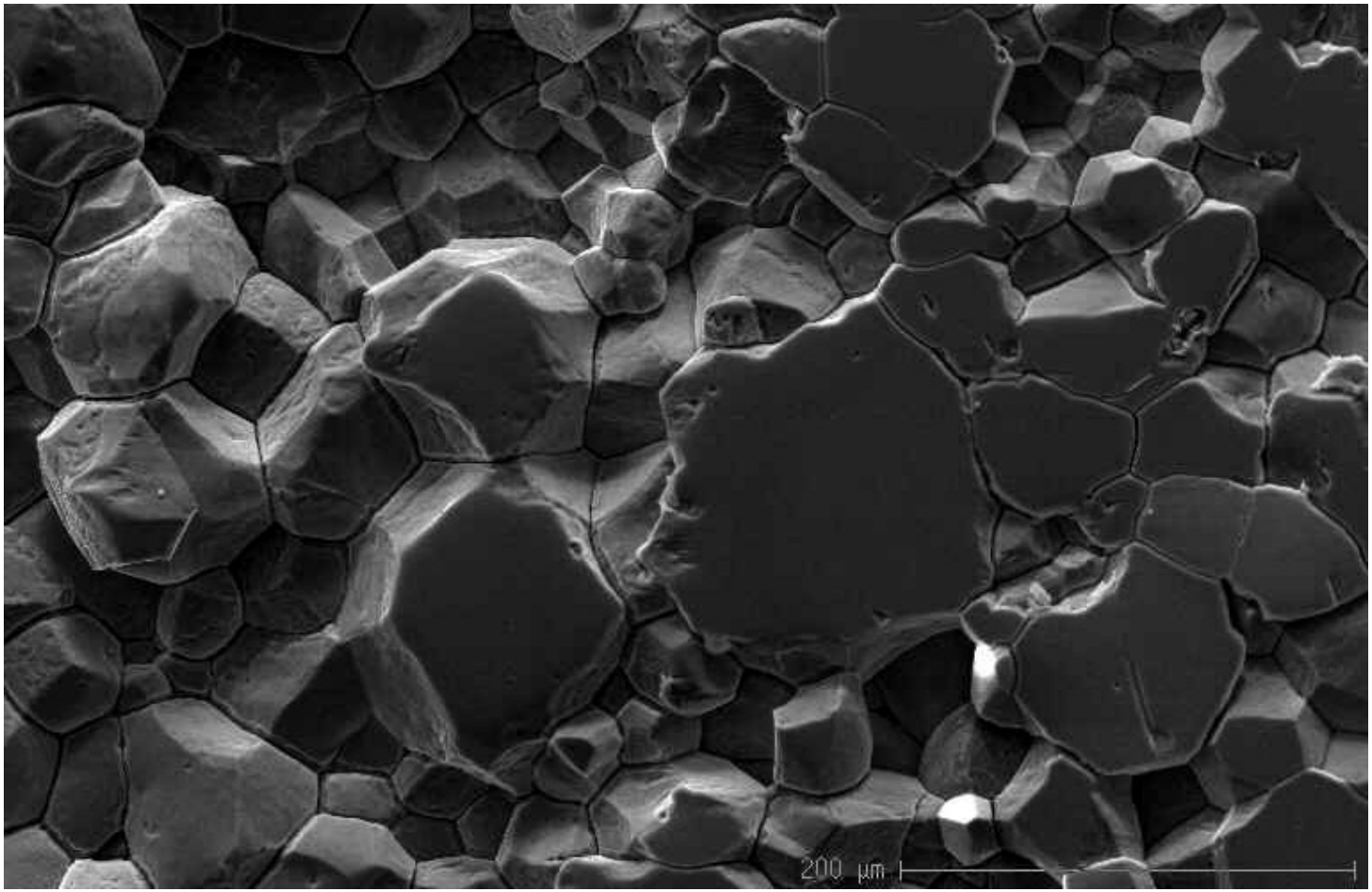
Aluminium alloy production in a nutshell

Aluminium alloys are created in the following way:

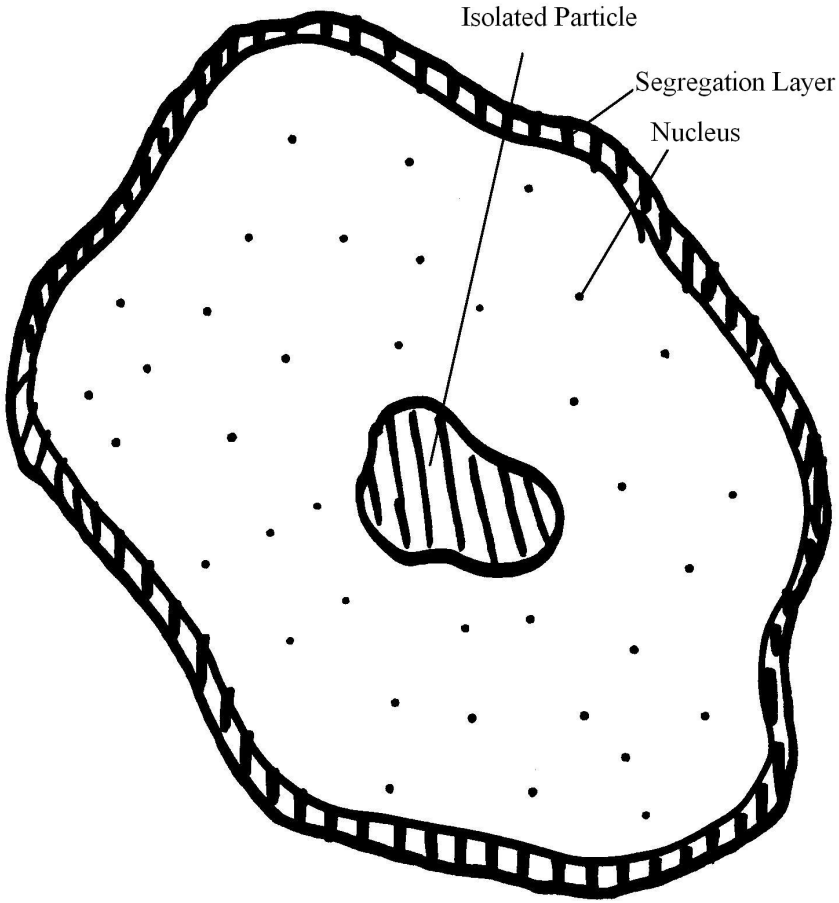
- Primary aluminium is melted
- Necessary alloying elements are added (i.e. Copper, Silicon, Magnesium)
- The liquid material is cast into a mould and left to solidify

Due to the nature of the solidification process the material is subject to structural changes.

Aluminium alloys consist of microscopic grains



Schematic view of the inside of a grain



- Presence of isolated particles and segregation layers that have high concentrations of alloying elements.
- The aluminium-rich phase is supersaturated.

The homogenization process

- After casting the alloy is not suitable for further processing (rolling, extrusion)
- Properties of the alloy may be improved by use of a heat treatment.
- Heating the material to just below the melting point results in:
  - Dissolution of isolated particles and segregation layers
  - Precipitation of new particles from the supersaturated phase

Different models can be used to simulate this behaviour

Traditionally, dissolution and precipitation are handled separately by different models:

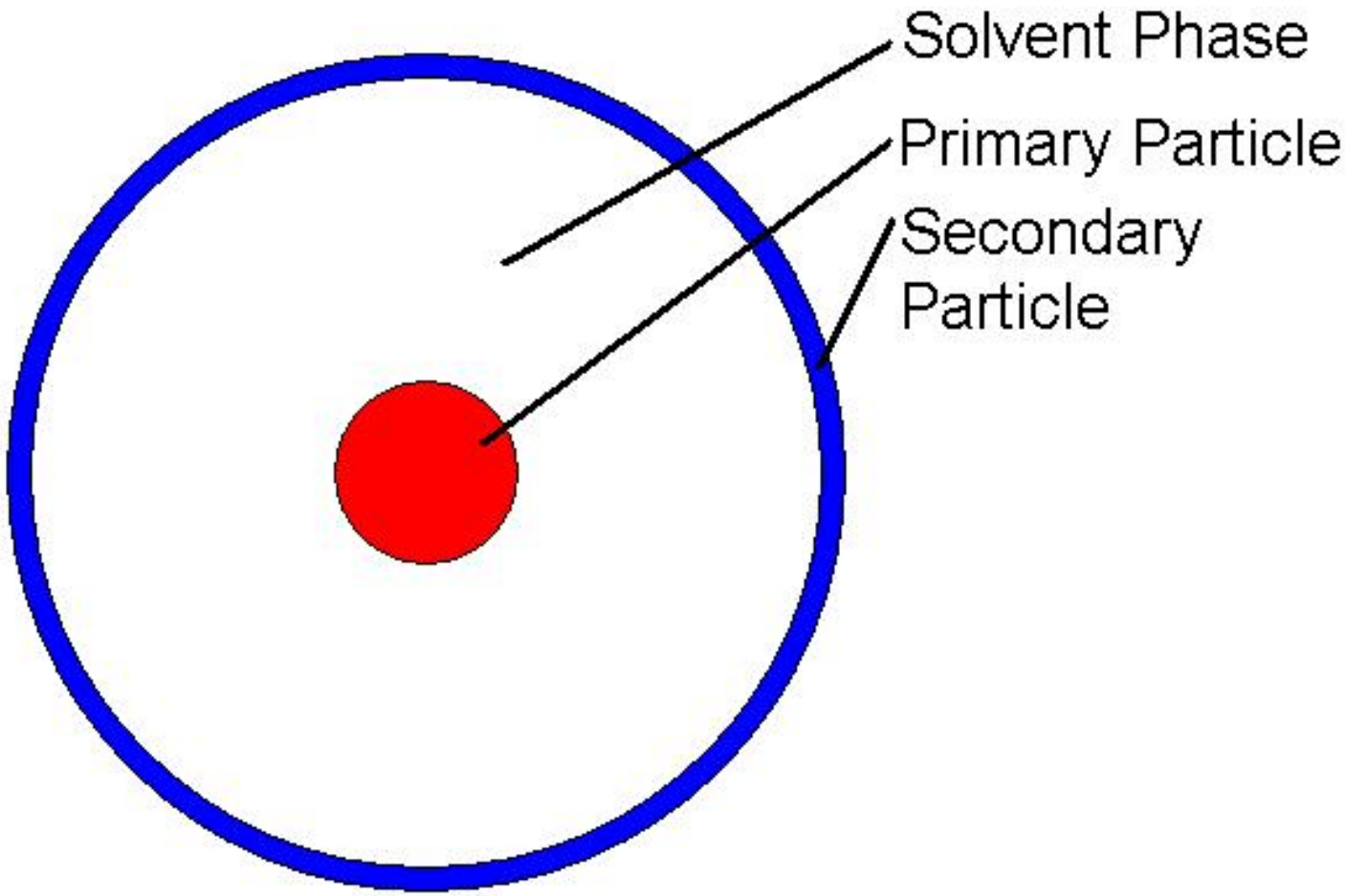
- A model which handles dissolution of one or two relatively large (micrometer) particles inside a specified finite grain geometry.
- A model which handles precipitation of millions of very small (nanometer) particles inside an infinite volume of material using classical nucleation theory.

Currently, only the dissolution model is used by Corus.

What Are the Goals of This Project?

1. To extend the model now in use at Corus to accommodate for the presence of nanometer-scale particles.
2. To investigate the influence of the presence of these particles on the dissolution of micrometer-scale particles.

Dissolution of particles inside a grain



Assumptions for the dissolution model

1. The concentration of components is “low”.
2. Diffusion only takes place inside the solvent phase. Particles are diffusion-free.
3. Particles are assumed to be of uniform, stoichiometric composition. ($A^l B^m C^n$)
4. Thermodynamic equilibrium is maintained at all times at the moving boundaries.

Component transfer inside the primary phase

Diffusion is governed by Fick's second law:

$$\frac{\partial c_p}{\partial t} = \frac{D_p}{r^a}\frac{\partial}{\partial r}\left\{ r^a \frac{\partial c_p}{\partial r} \right\}.$$

Initial condition:

$$c_p(x,0) = c^0(x) \qquad \text{for } x \in \Omega(0).$$

Boundary conditions:

$$c_p(S_1(t),t) = c_p^I(t) \qquad \text{(moving)}$$

$$\frac{\partial c_p(M_2,t)}{\partial r} = 0 \qquad \text{(fixed)}$$

Handling the moving boundaries

Movement of the boundary is prescribed by

$$\frac{dS_1}{dt} = \frac{D_p}{c_p^{\text{part}} - c_p^I} \frac{\partial c_p}{\partial r}(S_1(t), t)$$

so due to stoichiometry

$$\frac{D_B}{c_B^{\text{part}} - c_B^I} \frac{\partial c_B}{\partial r}(S_1(t), t) = \frac{D_C}{c_C^{\text{part}} - c_C^I} \frac{\partial c_C}{\partial r}(S_1(t), t)$$

Because of thermodynamic equilibrium at the interface

$$\left(c_B^I\right)^m \cdot \left(c_C^I\right)^n = K(T)$$

Solving the dissolution problem numerically

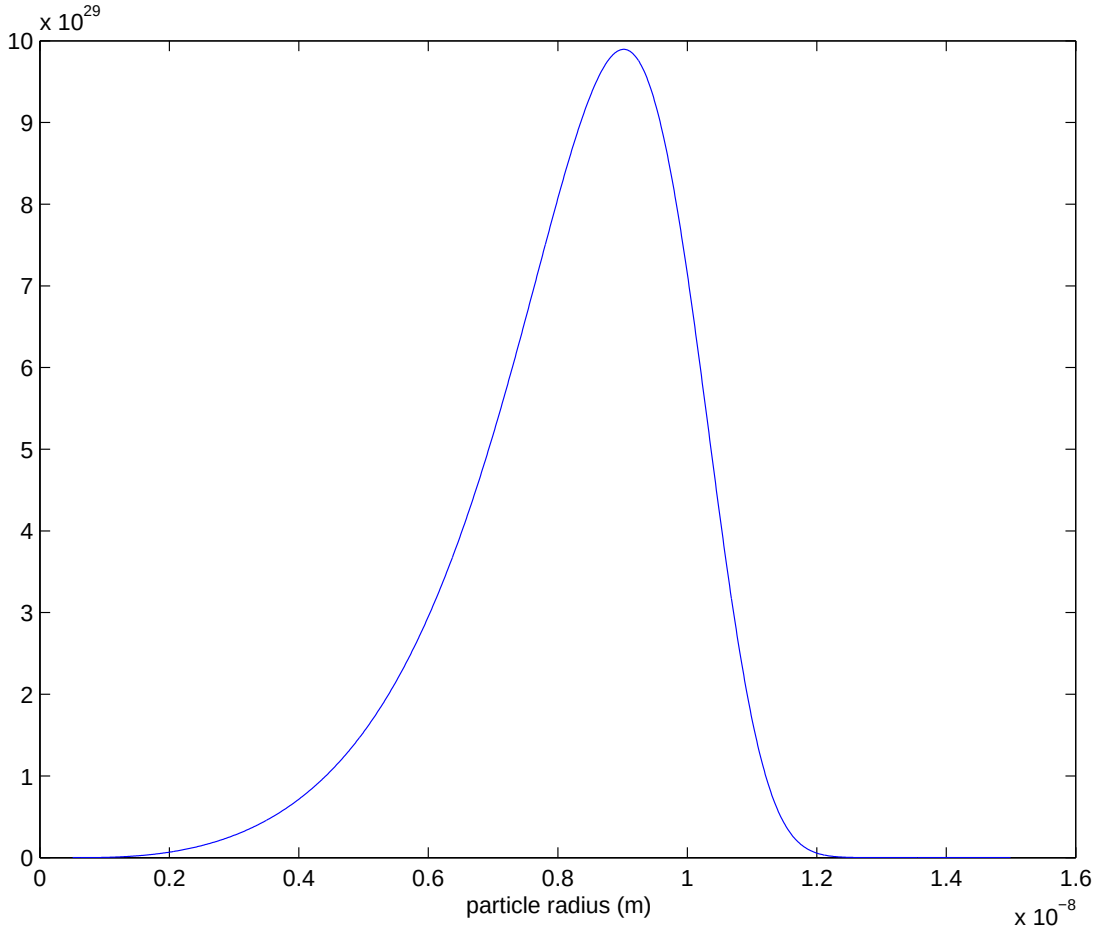
Algorithm outline:

1. Compute the concentration profiles by solving the non-linear problem using finite volumes and newton-raphson.
2. Predict the positions of the moving boundaries at the new time-step.
3. Redistribute the grid such that the boundaries are nodal points.
4. Repeat from step 1 for as long as desired.

Precipitation of particles in a supersaturated phase

- Tracking millions of particles inside a grain is infeasible.
- We will track classes of particles based on their radius using a particle size distribution function.

Example particle size distribution



Assumptions for the precipitation model

1. Precipitates are assumed to be stoichiometric.
2. Precipitates are in thermodynamic equilibrium at all times.
3. All particles are assumed spherical.
4. A “steady-state diffusion field” is assumed around the particles, i.e. Fick’s first law of thermodynamics applies.
5. Soft impingement does not occur. Diffusion fields of particles do not interact. This implies a dilute concentration of solute.

Nucleation

The number of nuclei produced is given by

$$J = J_0 \exp\left(-\frac{\Delta G^*_{\text{het}}}{RT}\right) \exp\left(-\frac{Q_d}{RT}\right)$$

Energy barrier for nucleation:

$$\Delta G^*_{\text{het}} = \frac{(A_0)^3}{(RT)^2[\ln(C_m/C_e)]^2}$$

Growth rate

Since we have assumed a steady-state diffusion field

$$v = \frac{dr}{dt} = \frac{C_m - C_i}{C_p - C_i}\frac{D}{r}$$

Because of the Gibbs-Thomson effect we have

$$C_i = C_e \exp\left(\frac{2\sigma V_m}{rRT}\right)$$

Critical radius:

$$r^* = \frac{2\sigma V_m}{RT}\left(\ln\left(\frac{C_m}{C_e}\right)\right)^{-1}$$

Particle size distribution

Particle size distribution is defined as

$$\#\ \text{particles}/m^3 \text{ with } r_{\min} \leq \text{particle radius} \leq r_{\max} = \int_{r=r_{\min}}^{r_{\max}} \varphi(r,t)\, dr.$$

The particle size distribution is controlled by the following differential equation

$$\frac{\partial \varphi(r,t)}{\partial t} = -\frac{\partial(\varphi(r,t)v(r,t))}{\partial r} + S(r,t)$$

This a convection equation with only outflow boundaries. Therefore it is sufficient to supply an initial size distribution

$$\varphi(r,0) = \varphi^0(r)$$

Particle volume fraction

The particle volume fraction is defined as the relative amount of volume occupied by the precipitates

$$f = \frac{C_0 - C_m}{C_p - C_m}. \tag{1}$$

Conservation of mass implies the following relation between the volume fraction and the size distribution

$$f = \int_{r=0}^{\infty} \frac{4}{3}\pi r^3 \varphi \, dr.$$

Solving the precipitation problem numerically

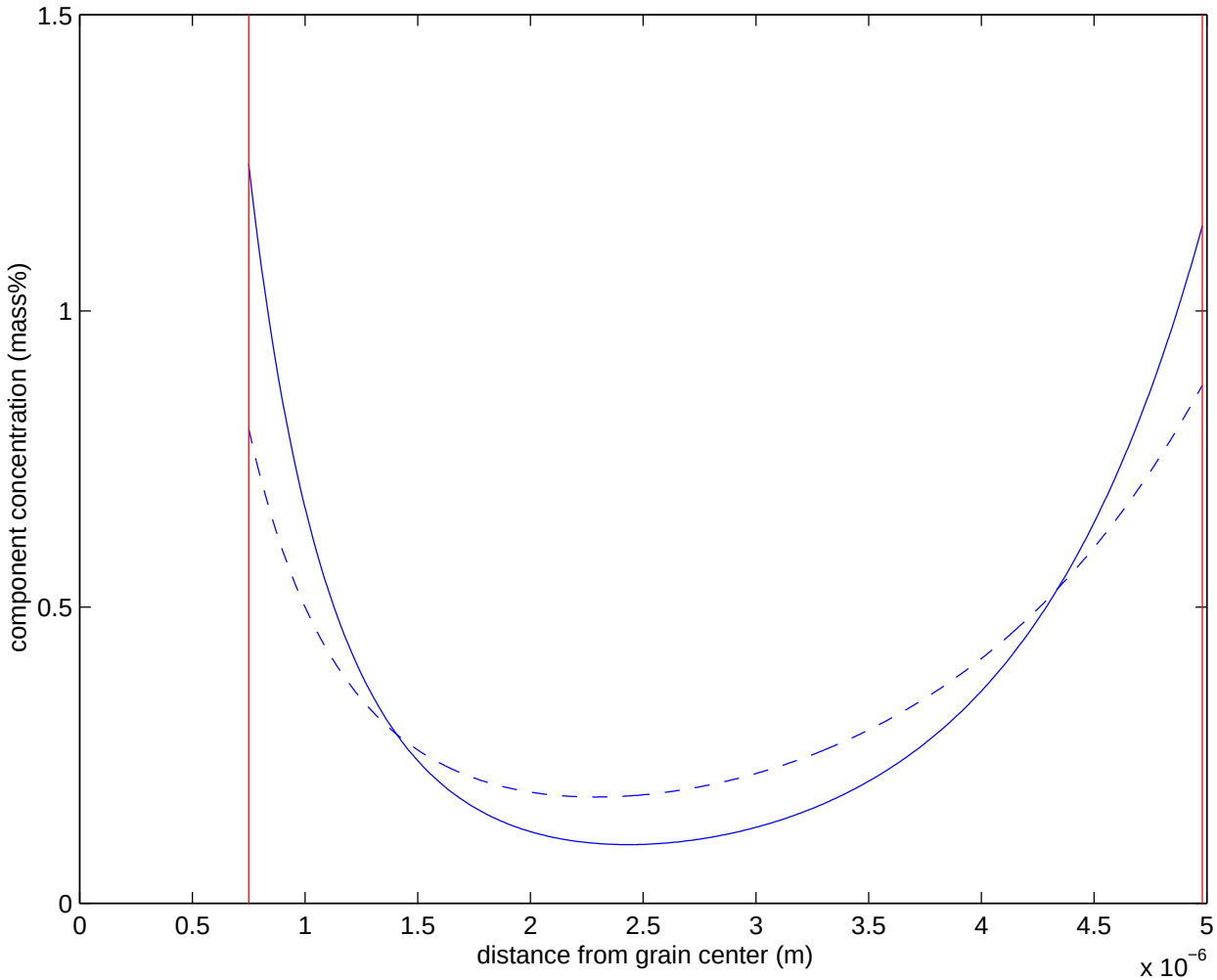
1. Calculate the nucleation rate, mean matrix concentration and velocity field from the particle size distribution.
2. Perform one implicit euler time step for the continuity equation (using finite volumes) to find the new size distribution.
3. Calculate and store statistics (e.g. volume fraction, mean radius etc.).
4. Repeat from step 1 until at end time.

Plans for the future

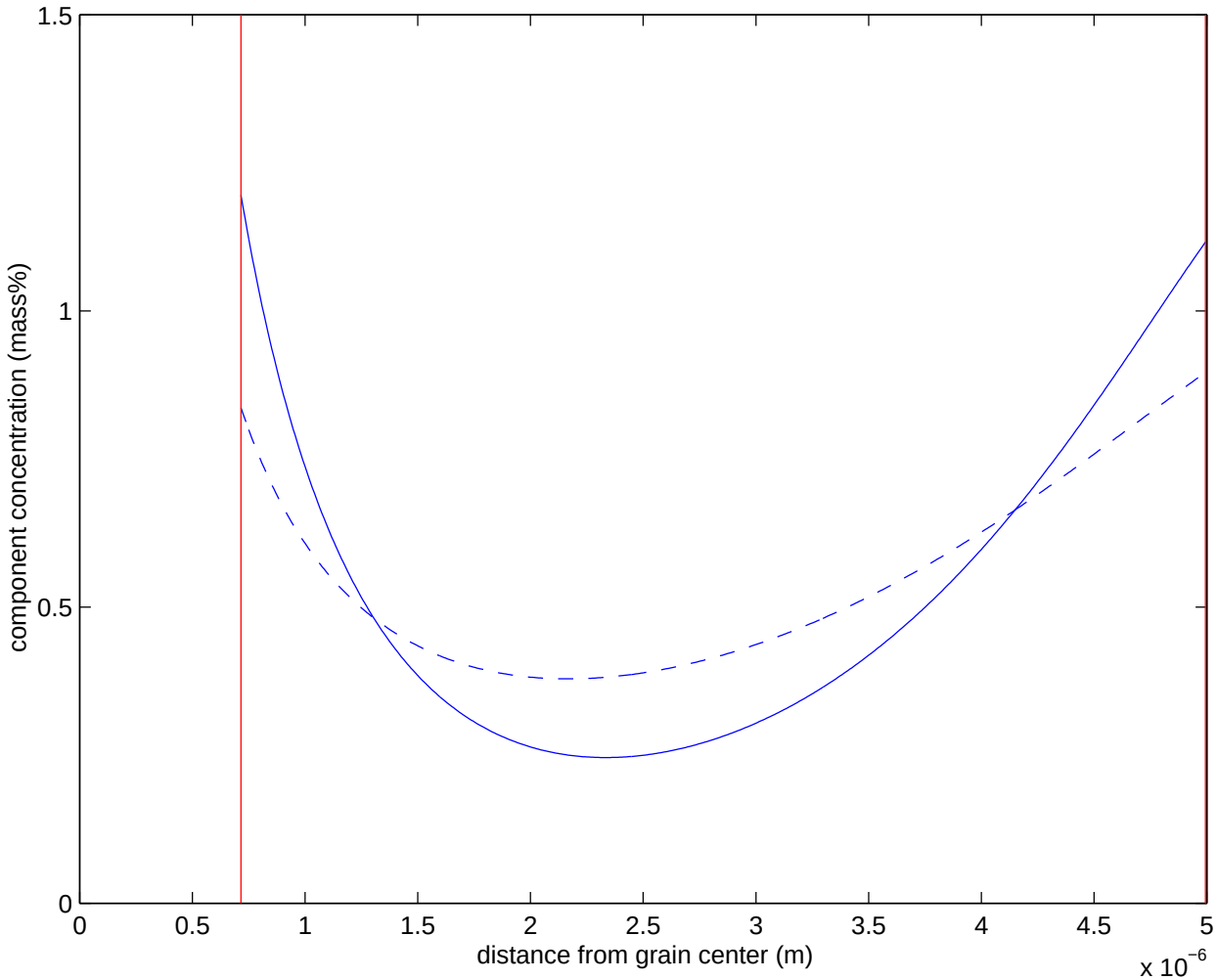
- Expand nucleation model to multi-component systems
- Combine dissolution and precipitation in one model
- Perform a parameter study

Questions?

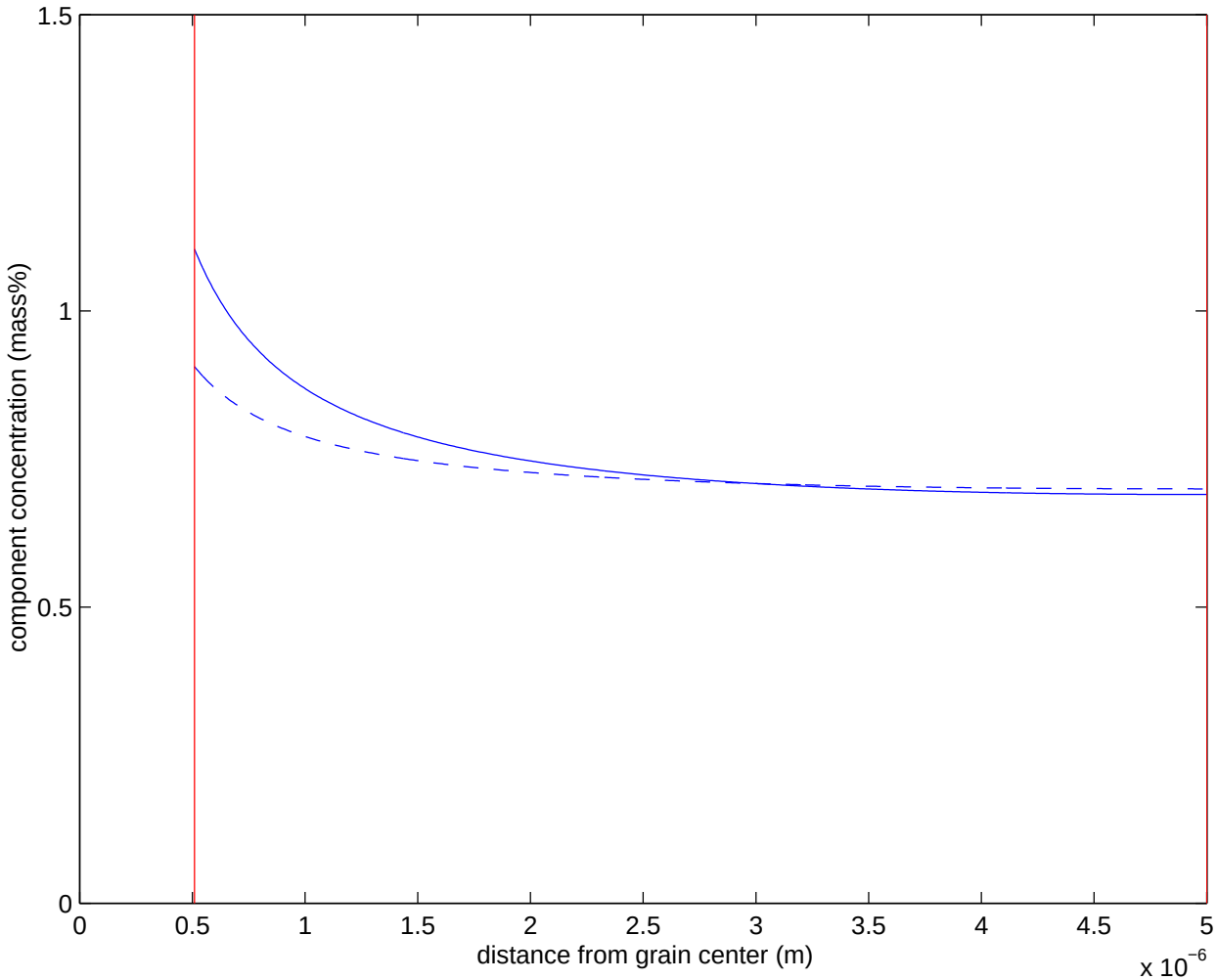
Dissolution Example: $t = 5$ s



Dissolution Example: $t = 10$ s



Dissolution Example: $t = 100$ s



Dissolution Example: $t = 250$ s