



UNIVERSITY OF NOVA GORICA

MODELLING OF SOLIDIFICATION WITH SOLID PHASE MOVEMENT

Gregor Košak

Advisor: prof. dr. Božidar Šarler

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Outline

- Goals
- Physical phenomena
- Modelling principles
- Physical system
- Derivation of governing equations by volume averaging and mixture theory
- Modeling of microstructure formation
- Coupling of micro and macro equations
- Computational model
- Conclusions
- Literature review



Goals

- Overview of the literature on modelling of solidification systems
- Physical modelling of solidification systems on the macroscopic scale
- Physical modelling of solidification systems on the microscopic scale
- Development of the multiscale and multiphysics equations that will be used in a Ph. D. project

Physical phenomena



Melting: solid-liquid



Solidification: liquid-solid

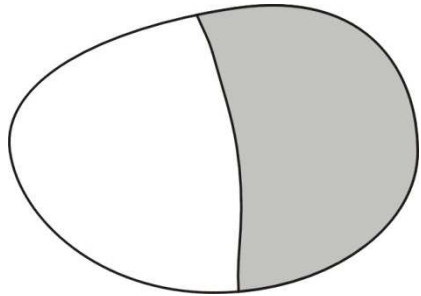


Crystal growth: gas-solid

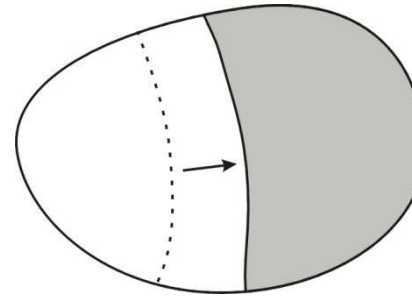


Allotropic transformations: solid-solid

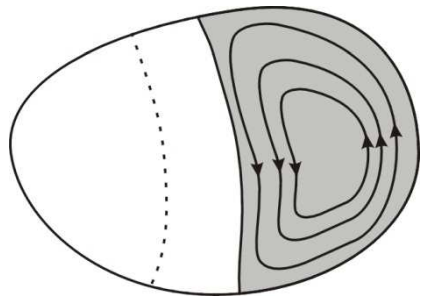
Physical phenomena



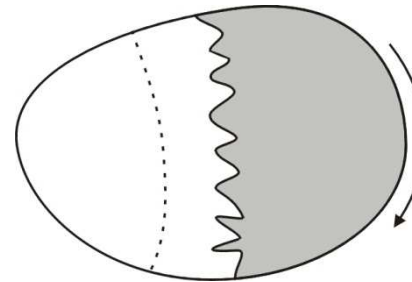
jump of
physical
properties



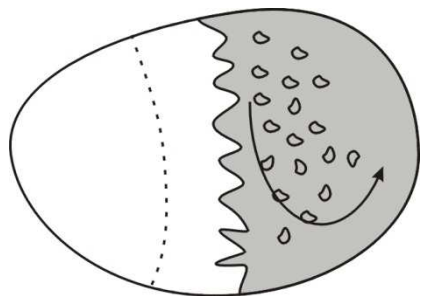
moving boundary



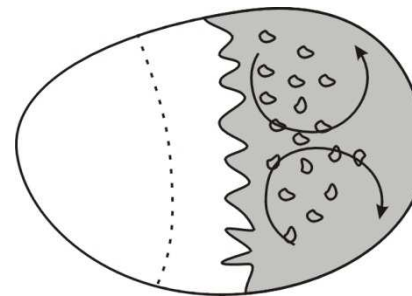
bulk
convection



surface tension
convection



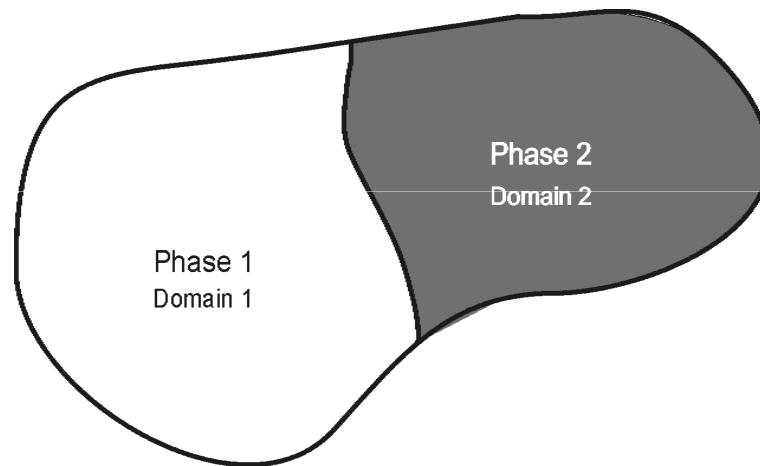
dispersed
phase



double-diffusive
convection

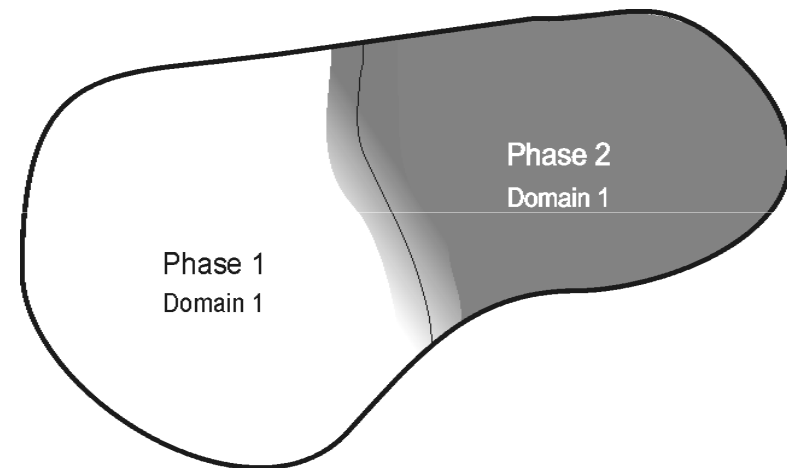
Physical phenomena

two-domain



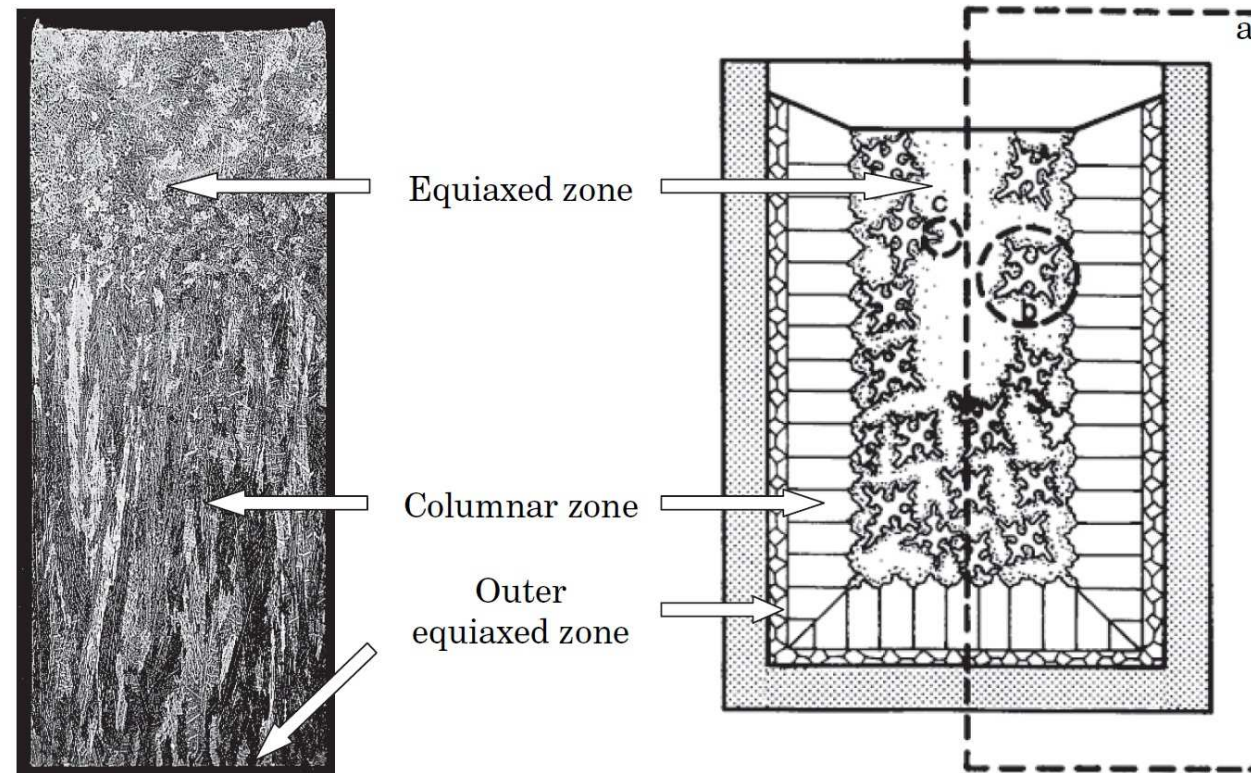
moving boundary

one-domain



moving transformed into high nonlinearity

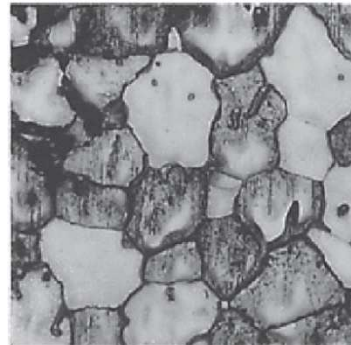
Physical phenomena



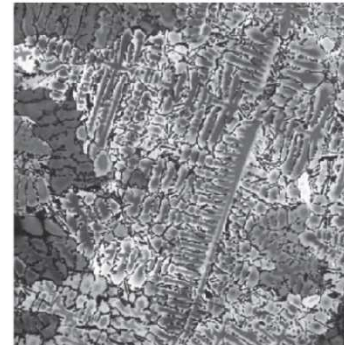
The grain structure as observed in a directionally solidified Al-7wt%Si casting (left) and solidification process is illustrated for a 2D casting (right). The outer equiaxed, columnar and (inner) equiaxed zones are indicated.

Physical phenomena

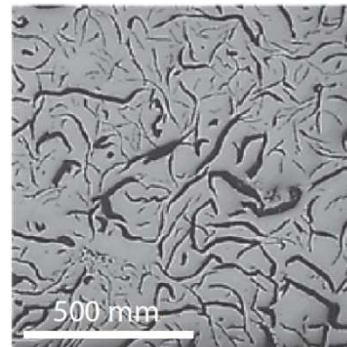
Equiaxed grains growing in a uniform temperature field



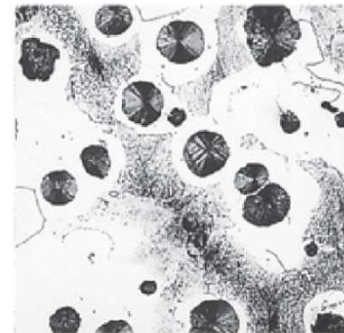
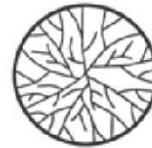
(a) Globulitic grains



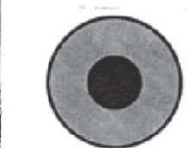
(b) Dendritic grains



(c) Gray cast iron



(d) Nodular cast iron



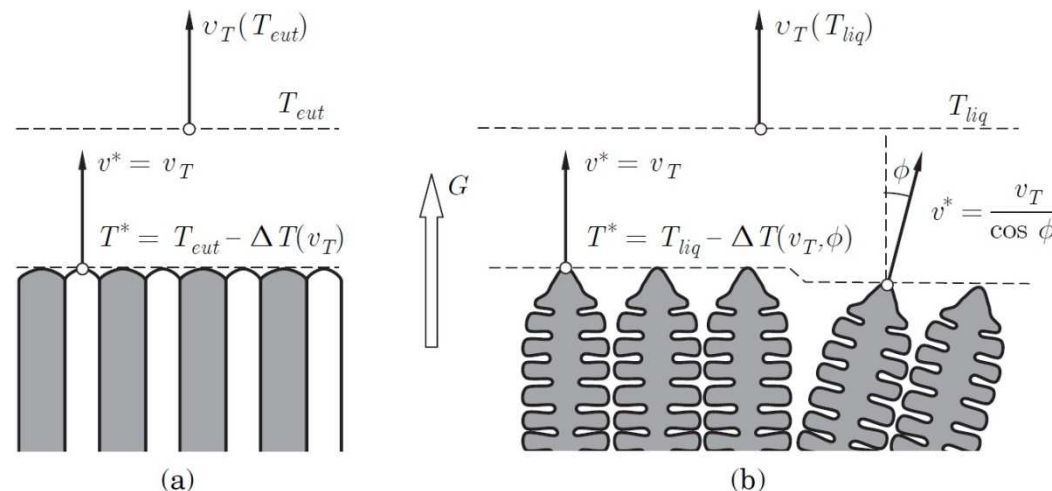
Heterogeneous nucleation

Equiaxed grain types frequently encountered in solidification: (a) globulitic grains in Al-1wt%Cu (grain size $100\mu\text{m}$), (b) dendritic grains in an Al-7wt%Si alloy (grain size 2mm), (c) gray cast iron, and (d) nodular cast iron (typical graphite nodule size $50\mu\text{m}$)

Physical phenomena

Columnar grains

- Dendrites whose preferred direction is inclined with respect to G must grow faster in order to maintain their relative tip positions
- Tips of the inclined dendrites lie slightly behind those of well-aligned dendrites
- Growth competition among columnar dendrites results in a natural selection of grains with a small angle ϕ



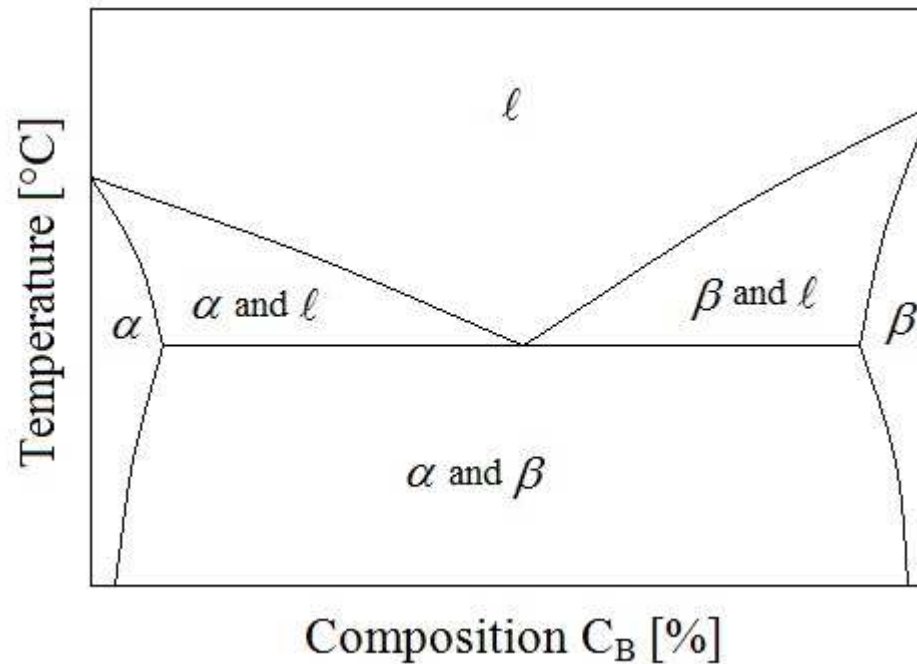
Velocities of (a) eutectic isotherm and eutectic front, and (b) liquidus isotherm and dendrite tips. Because dendrites are constrained to grow along well-defined directions, their velocity, and thus their undercooling, depend on their angle of inclination with respect to the thermal gradient.

Modeling principles

- Deterministic and stochastic
- Macro level
 - Mixture theory
 - Volume averaging
 - Ensemble averaging
- Micro level
 - Monte Carlo methods
 - Cellular automata method (Point automata)

Physical system

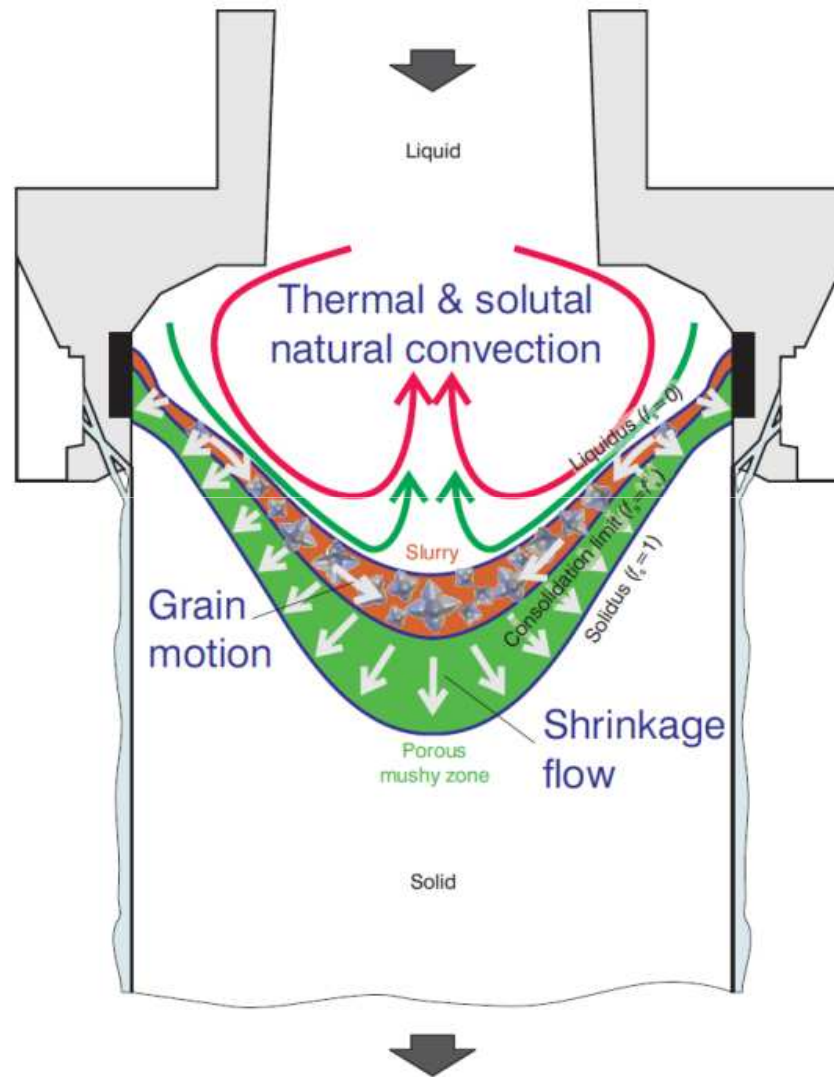
- Cartesian coordinate system
- Continuum mechanics
- Two-phase, binary alloy system
- Newtonian fluid
- Binary eutectic phase diagram:



Physical system

- Double diffusive convection: convection depends on temperature and concentration
- Stationary solid phase
- Moving solid phase
- Slurry flow regime
 - Volume fraction of the solid phase g_s smaller or equal than a predefined packing fraction g_s^c
- Porous flow regime
 - Volume fraction of the solid phase g_s greater than a predefined packing fraction g_s^c

Physical system

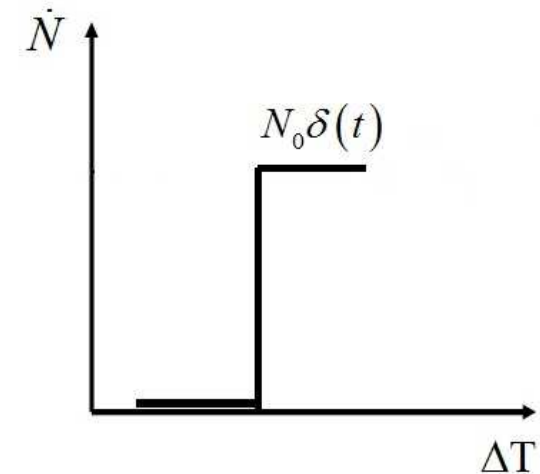


Example of industrial solidification system: DC casting of aluminium alloys

Physical system

- Creation of clusters: embryos and nuclei
- Homogeneous nucleation: clusters are assumed to appear spontaneously in a melt free of any impurities
- Heterogeneous nucleation: the clusters form preferentially
 - on foreign particles in the melt, or at interfaces (melt-container)
- Nucleation model:

$$\dot{N} = \begin{cases} N_0 \delta(t) & \text{if } T < T_{nucl} \text{ and } \int_0^t \dot{N} dt = 0 \\ N_0 \delta(t) & \text{if } T < T_{nucl} \text{ and } N = 0 \\ 0 & \text{else} \end{cases}$$



Physical system

- Microscopic conservation equations:

Mass:
$$\frac{\partial}{\partial t} \rho_k + \nabla \cdot (\rho_k \mathbf{v}_k) = 0$$

Momentum:
$$\frac{\partial}{\partial t} (\rho_k \mathbf{v}_k) + \nabla \cdot (\rho_k \mathbf{v}_k \mathbf{v}_k) = -\nabla p + \nabla \cdot \boldsymbol{\tau}_k + \mathbf{b}_k$$

Energy:
$$\frac{\partial}{\partial t} (\rho_k h_k) + \nabla \cdot (\rho_k h_k \mathbf{v}_k) = -\nabla \cdot \mathbf{q}_k$$

Species:
$$\frac{\partial}{\partial t} (\rho_k C_k) + \nabla \cdot (\rho_k C_k \mathbf{v}_k) = -\nabla \cdot \mathbf{j}_k$$

Physical system

- Microscopic interphase balances:
- Mass balance:

$$(\rho_\ell - \rho_s) \mathbf{v}^* \cdot \mathbf{n} = \rho_\ell \mathbf{v}_\ell^* \cdot \mathbf{n} - \rho_s \mathbf{v}_s^* \cdot \mathbf{n}$$

- Momentum balance:

$$-\mathbf{\Gamma}_s^{\sigma^*} + \mathbf{\Gamma}_\ell^{\sigma^*} = -\mathcal{S}_V \langle 2\gamma_{sl} \bar{\mathbf{k}}\mathbf{n} \rangle^* - \mathcal{S}_V \langle \nabla_{surf} \gamma_{sl} \rangle^*$$

- Energy balance (Stefan condition):

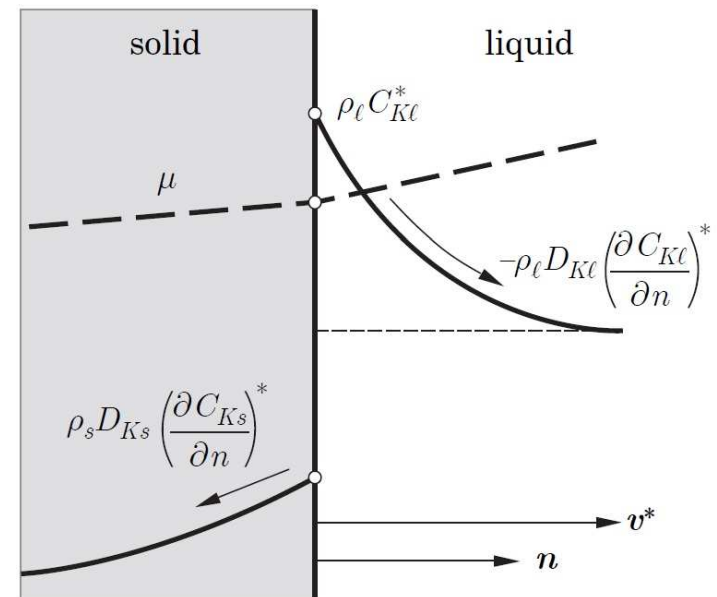
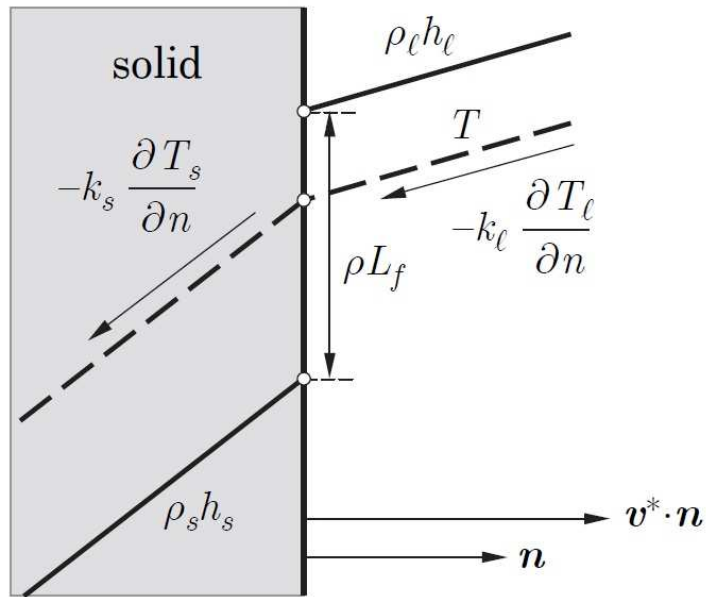
$$\rho_s L_f \mathbf{v}^* \cdot \mathbf{n} = \left(k_s \frac{\partial T_s}{\partial n} \right)^* - \left(k_\ell \frac{\partial T_\ell}{\partial n} \right)^*$$

- Solute balance:

$$\rho_s (1 - k_{OK}) C_{K\ell}^* (\mathbf{v}^* - \mathbf{v}_s^*) \cdot \mathbf{n} = \rho_s D_{Ks} \left(\frac{\partial C_{Ks}}{\partial n} \right)^* - \rho_\ell D_{K\ell} \left(\frac{\partial C_{K\ell}}{\partial n} \right)^*$$

Physical system

- Microscopic interphase balances:



Derivation of governing equations by volume averaging and mixture theory

Mixture continuum model

- The development of conservation equations from classical mixture theory is based on the following principles:
 - mixture components may be viewed as isolated subsystems, if interactions with other mixture components are properly treated
 - all properties of the mixture are mathematical consequences of the component properties
 - the mean collective mixture behavior is governed by equations similar to those governing the individual properties
- The partial density of phase k is

$$\bar{\rho}_k = g_k \rho_k$$

- Mixture density and mass averaged velocity:

$$\rho = \sum_k \bar{\rho}_k \qquad \mathbf{v} = \frac{1}{\rho} \sum_k \bar{\rho}_k \mathbf{v}_k$$

Derivation of governing equations by volume averaging and mixture theory

Mixture continuum model

- Mass balance:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

- The continuum equation governing the conservation of momentum can be obtained by summing over each phase

$$\begin{aligned} \frac{\partial}{\partial t} \left(\sum_k \bar{\rho}_k \mathbf{v}_k \right) + \nabla \cdot \left(\sum_k \bar{\rho}_k \mathbf{v}_k \mathbf{v}_k \right) = \\ \nabla \cdot \left(\sum_k g_k \boldsymbol{\tau}_k \right) - \frac{\partial}{\partial x} \left(\sum_k g_k p_k \right) + \sum_k (\bar{\rho}_k B_k) + F \end{aligned}$$

- In a Newtonian fluid, the relation between the shear stress and the velocity gradient is linear, the constant of proportionality being the coefficient of viscosity:

$$\boldsymbol{\tau} = \mu \nabla \mathbf{v}$$

Derivation of governing equations by volume averaging and mixture theory

Mixture continuum model

- The drag interaction term can be modeled by Darcy's law:

$$f = \frac{\mu_\ell}{K} \mathbf{v}$$

- Final momentum equation is:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \mu_\ell \nabla^2 \mathbf{v} - \frac{\mu_\ell}{K} \mathbf{v} + \tilde{\rho} \mathbf{g}$$

- Energy balance:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \mathbf{v}) = \nabla \cdot (k \nabla T)$$

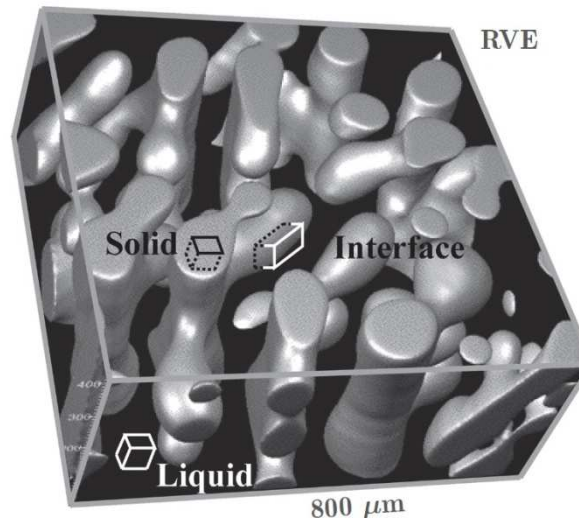
- Solute balance:

$$\frac{\partial}{\partial t}(\rho C) + \nabla \cdot (\rho C \mathbf{v}) = \nabla \cdot (\rho D \nabla C)$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaging definitions

- Consider the volume element which is located in the mushy zone
- The volume element is assumed to be sufficiently large to accurately represent the local structure at the mesoscopic length scale, yet small enough that important variations in the temperature, enthalpy and volume fraction of the solid are resolved for the problem of interest
- We refer to this volume as a 'Representative Volume Element' or RVE



Derivation of governing equations by volume averaging and mixture theory

Volume averaging definitions

- The macroscopic conservation equations for each phase are obtained by averaging the microscopic equations over the volume, V_R
- The volume average of any quantity in phase k is defined as

$$\langle \psi \rangle = \frac{1}{V_R} \int_{V_R} \psi dV$$

- The averaging process is assumed to satisfy the following properties:

$$\langle \psi + \phi \rangle = \langle \psi \rangle + \langle \phi \rangle \qquad \left\langle \frac{\partial \psi}{\partial x_i} \right\rangle = \frac{\partial \langle \psi \rangle}{\partial x_i}$$

$$\langle \langle \psi \rangle \phi \rangle = \langle \psi \rangle \langle \phi \rangle$$

$$\langle \text{const} \rangle = \text{const}$$

$$\left\langle \frac{\partial \psi}{\partial t} \right\rangle = \frac{\partial \langle \psi \rangle}{\partial t}$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaging definitions

- To be able to average equations over each of the interdispersed phases the phase function $X_k(\mathbf{x}, t)$ is introduced, being equal to one in phase k and zero otherwise,

$$X_k(\mathbf{x}, t) = \begin{cases} 1 & \text{where } \mathbf{x} \text{ is in phase } k \text{ at time } t \\ 0 & \text{elsewhere} \end{cases}$$

- The quantity in phase k is expressed as $\psi_k = X_k \psi$
- The phase function $X_k(\mathbf{x}, t)$ is a generalised function and the properties of averaging of derivatives do not apply for it
- The volume average of the phase function is equal to the phase volume fraction

$$\langle X_k \rangle = \frac{1}{V_R} \int_{V_R} X_k dV = \frac{V_k}{V_R} = g_k; \quad \sum_k g_k = 1$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaging definitions

- The volume average of quantity ψ in phase k over the volume V_R is

$$\langle \psi_k \rangle = \langle X_k \psi \rangle = \frac{1}{V_R} \int_{V_R} X_k \psi dV$$

- The intrinsic volume average, i.e. the average value of the quantity inside phase k is

$$\langle \psi_k \rangle^k = \langle X_k \psi \rangle^k = \frac{1}{V_k} \int_{V_k} X_k \psi dV = g_k \langle \psi_k \rangle$$

- The average of the product is

$$\langle \psi_k \phi_k \rangle = \langle X_k \psi \phi \rangle = \langle \psi_k \rangle \langle \phi_k \rangle^k + \langle \hat{\psi}_k \hat{\phi}_k \rangle$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaging definitions

- The average of the time derivative is

$$\left\langle \left(\frac{\partial \psi}{\partial t} \right)_k \right\rangle = \left\langle \frac{\partial \psi}{\partial t} X_k \right\rangle = \frac{\partial}{\partial t} \left(g_k \langle \psi_k \rangle^k \right) + \frac{1}{V_R} \int_{A_k} \psi_k \mathbf{w}_i \cdot \mathbf{n}_k dA$$

- where \mathbf{w}_i is the velocity of the phase interface.
- The average of the gradient is

$$\langle \nabla \psi_k \rangle = \nabla \langle \psi_k \rangle - \frac{1}{V_R} \int_{A_k} \psi_k \mathbf{n}_k dA = g_k \nabla \langle \psi_k \rangle^k - \frac{1}{V_R} \int_{A_k} \hat{\psi}_k \mathbf{n}_k dA.$$

- The average of the divergence is

$$\langle (\nabla \cdot \boldsymbol{\psi})_k \rangle = \langle X_k \nabla \cdot \boldsymbol{\psi} \rangle = g_k \nabla \cdot \langle \boldsymbol{\psi}_k \rangle^k + \langle \boldsymbol{\psi}_k \rangle^k \cdot \nabla g_k - \frac{1}{V_R} \int_{A_k} \hat{\boldsymbol{\psi}}_k \mathbf{n}_k dA.$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- Hypotheses:

- the densities of both phases are assumed to be equal and constant, except for buoyancy – Boussinesq approximation, $\rho_s = \rho_\ell = \rho$
- laminar flow and constant viscosity μ_ℓ
- solute diffusion in the liquid and solid at the macroscopic scale is neglected
- local thermodynamic equilibrium is assumed, with perfect solute diffusion in both phases (lever rule)
- the mushy zone is an isotropic porous medium whose permeability K is defined by Carman-Kozeny relation
- constant thermal conductivity
- constant heat capacity
- saturated medium ($g_s + g_\ell = 1$)
- thermal equilibrium between phases ($\langle T_s \rangle^s = \langle T_\ell \rangle^\ell = T$)
- fixed solid phase ($\langle \mathbf{v}_s \rangle^s = 0$)

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- The averaged mass balance for phase k is

$$\frac{\partial}{\partial t}(g_k) + \nabla \cdot (g_k \langle \mathbf{v}_k \rangle^k) = \frac{1}{\rho}(\Gamma_k + \Phi_k)$$

- The averaged momentum balance for phase k is

$$\begin{aligned} \frac{\partial}{\partial t}(g_k \langle \mathbf{v}_k \rangle^k) + \nabla \cdot (g_k \langle \mathbf{v}_k \rangle^k \langle \mathbf{v}_k \rangle^k) &= -\frac{g_k}{\rho} \nabla p_k + \frac{1}{\rho} \nabla \cdot (g_k \langle \boldsymbol{\tau}_k \rangle^k) \\ &+ \frac{g_k}{\rho} \rho_k^b \mathbf{g} + \frac{1}{\rho} (\mathbf{M}_k^d + \mathbf{M}_k^\Gamma + \mathbf{M}_k^\Phi) \end{aligned}$$

- Phase change and grain nucleation are usually neglected

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- The averaged solute mass balance for species i in phase k is

$$\frac{\partial}{\partial t} \left(g_k \langle C_k^i \rangle^k \right) + \nabla \cdot \left(g_k \langle C_k^i \rangle^k \langle \mathbf{v}_k \rangle^k \right) = \frac{1}{\rho} \left(J_k^{i,j} + J_k^{i,\Gamma} + J_k^{i,\Phi} \right)$$

- The averaged heat balance for phase k is

$$\begin{aligned} \frac{\partial}{\partial t} \left(g_k \langle h_k \rangle^k \right) + \nabla \cdot \left(g_k \langle h_k \rangle^k \langle \mathbf{v}_k \rangle^k \right) &= \frac{1}{\rho} \nabla \cdot \left(g_k k_k \langle \nabla T_k \rangle^k \right) \\ &+ \frac{1}{\rho} \left(Q_k^j + Q_k^\Gamma + Q_k^\Phi \right) \end{aligned}$$

- The interphase transfer of mass and solute and nucleation require additional modeling
- This information has been lost during the volume averaging process

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- The nucleation and phase change terms ($\mathbf{M}_k^\Phi \approx 0$ and $\mathbf{M}_k^\Gamma \approx 0$) are neglected
- The liquid phase is modeled as a Newtonian fluid and the tangential stress term is thus $\nabla \cdot (g_\ell \langle \boldsymbol{\tau}_\ell \rangle^\ell) = \nabla \cdot (\mu_\ell \nabla g_\ell \langle \mathbf{v}_\ell \rangle^\ell)$
- The interfacial momentum balance ($\mathbf{M}_\ell^d = -\mathbf{M}_s^d$) is applied and the phase change term is neglected ($\mathbf{M}_\ell^\Gamma \approx 0$)
- The solid phase momentum ($-g_s \nabla p + \mathbf{M}_s^d + g_s \mathbf{g} \rho_s^b = 0$) can be applied and we obtain

$$\frac{\partial}{\partial t} (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell) + \nabla \cdot (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell \langle \mathbf{v}_\ell \rangle^\ell) = -\nabla p + \nabla \cdot (\mu_\ell \nabla (g_\ell \langle \mathbf{v}_\ell \rangle^\ell)) + \tilde{\rho} \mathbf{g}$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- In the liquid momentum balance the interfacial drag force is modeled according to the Darcy model:

$$\mathbf{M}_k^d = -\frac{g_\ell^2 \mu_\ell}{K} \langle \mathbf{v}_\ell \rangle^\ell$$

- The momentum balance in the liquid phase in the porous region is thus

$$\begin{aligned} \frac{\partial}{\partial t} (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell) + \nabla \cdot (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell \langle \mathbf{v}_\ell \rangle^\ell) = \\ -g_\ell \nabla p + g_\ell \mu_\ell \nabla^2 \langle \mathbf{v}_\ell \rangle^\ell - \frac{g_\ell^2 \mu_\ell}{K} \langle \mathbf{v}_\ell \rangle^\ell + g_\ell \tilde{\rho} \mathbf{g} \end{aligned}$$

- The Kozeny–Carman equation is used to model the permeability of the columnar structure

$$K = \frac{g_\ell^2}{(1-g_\ell)^2} \frac{d_s^2}{\pi^2 k_K \tau^2}$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- In order to get the solution, we have to solve a set of equations

$$\nabla \cdot \langle \mathbf{v}_\ell \rangle^\ell = 0,$$

$$\frac{\partial}{\partial t} (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell) + \nabla \cdot (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell \langle \mathbf{v}_\ell \rangle^\ell) = -g_\ell \nabla p + g_\ell \mu_\ell \nabla^2 \langle \mathbf{v}_\ell \rangle^\ell - \frac{g_\ell^2 \mu_\ell}{K} \langle \mathbf{v}_\ell \rangle^\ell + g_\ell \tilde{\rho} \mathbf{g},$$

$$\rho \frac{\partial \langle h \rangle}{\partial t} + \nabla \cdot (\rho c_p \nabla T^\ell \cdot \langle \mathbf{v}_\ell \rangle^\ell) - \nabla \cdot (k \nabla T) = 0,$$

$$\rho \frac{\partial \langle C \rangle}{\partial t} + \nabla \cdot \langle C_\ell \rangle^\ell \cdot \langle \mathbf{v}_\ell \rangle^\ell = 0$$

- Density variation with temperature and composition:

$$\tilde{\rho} = \rho (1 - \beta_T (T - T_0) - \beta_C (\langle C_\ell \rangle^\ell - C_0))$$

- Enthalpies:

$$\langle h_s \rangle^s = c_p T \quad \langle h_\ell \rangle^\ell = c_p T + L \quad \langle h \rangle = c_p T + g_\ell L$$

- Microsegregation model (lever rule):

$$\langle C \rangle = g_\ell \langle C_\ell \rangle^\ell + g_s \langle C_s \rangle^s = (g_\ell + k_p (1 - g_\ell)) \langle C_\ell \rangle^\ell \quad T = T_f + m \langle C_\ell \rangle^\ell$$

Derivation of governing equations by volume averaging and mixture theory

Volume averaged model

- The initial and boundary conditions:

$$\langle \mathbf{v}_\ell \rangle^\ell (x=W, t) = \langle \mathbf{v}_\ell \rangle^\ell (y=H, t) = \langle \mathbf{v}_\ell \rangle^\ell (y=0, t) = 0$$

$$\frac{\partial}{\partial x} \langle \mathbf{v}_{\ell y} \rangle^\ell (x=0, t) = 0$$

$$\frac{\partial}{\partial x} T(x=W, t) = \frac{q}{\lambda} (T - T_{ext})$$

$$\frac{\partial}{\partial x} T(x=0, t) = \frac{\partial}{\partial y} T(y=0, t) = \frac{\partial}{\partial y} T(y=H, t) = 0$$

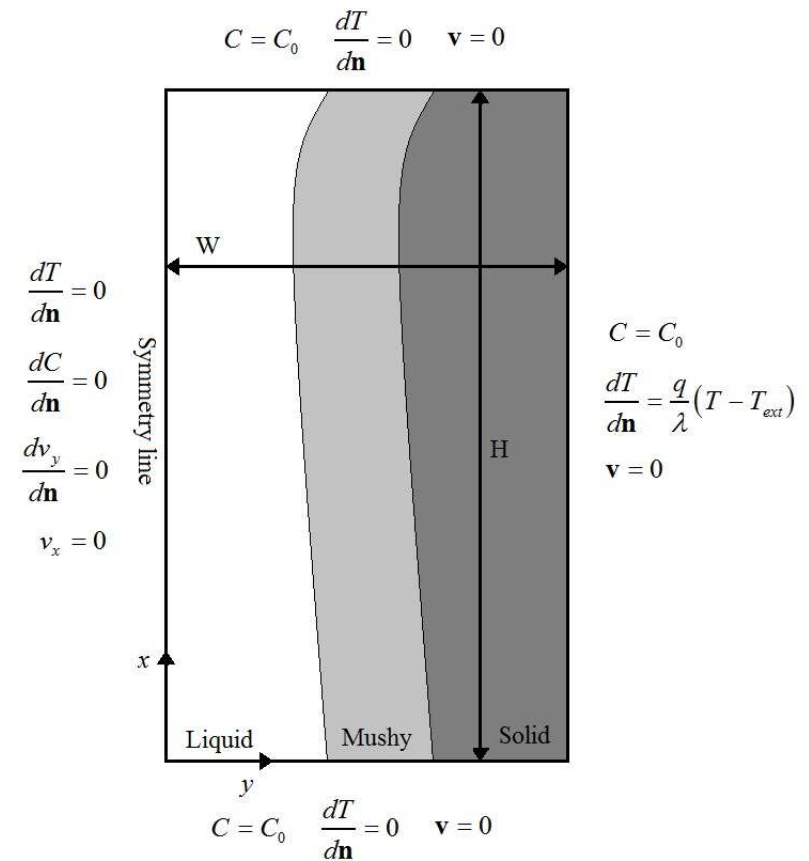
$$\frac{\partial}{\partial x} \langle C \rangle (x=0, t) = 0$$

$$\langle C \rangle (x=W, t) = \langle C \rangle (y=H, t) = \langle C \rangle (y=0, t) = C_0$$

$$\langle \mathbf{v}_\ell \rangle^\ell (\mathbf{p}, t=0) = 0$$

$$T(\mathbf{p}, t=0) = T_0$$

$$\langle C \rangle (\mathbf{p}, t=0) = C_0$$



Derivation of governing equations by volume averaging and mixture theory

Comparison of momentum equations

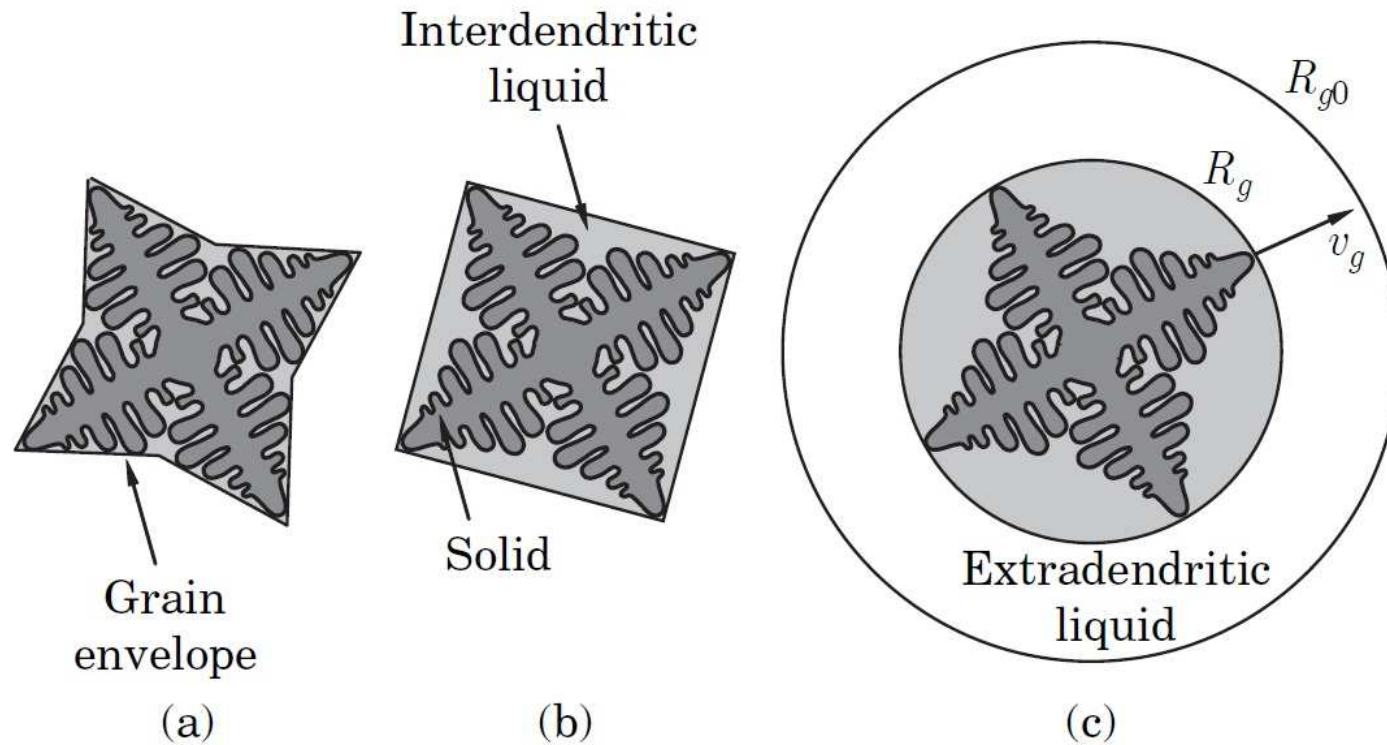
- Mixture continuum momentum equation:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \mu_\ell \nabla^2 \mathbf{v} - \frac{\mu_\ell}{K} \mathbf{v} + \tilde{\rho} \mathbf{g}$$

- Volume averaged momentum equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell) + \nabla \cdot (\rho g_\ell \langle \mathbf{v}_\ell \rangle^\ell \langle \mathbf{v}_\ell \rangle^\ell) = \\ -g_\ell \nabla p + g_\ell \mu_\ell \nabla^2 \langle \mathbf{v}_\ell \rangle^\ell - \frac{g_\ell \mu_\ell}{K} \langle \mathbf{v}_\ell \rangle^\ell + g_\ell \tilde{\rho} \mathbf{g} \end{aligned}$$

Modeling of microstructure formation



A 2D schematic of an equiaxed dendrite surrounded by a cruciform (a), square (b) and spherical envelope (c)

Modeling of microstructure formation

- Lever rule (equilibrium solidification model): complete mixing of solute in liquid and solid is assumed

$$f_s = \frac{1}{1-k_0} \frac{T_\ell - T}{T_m - T}; \quad T_s \leq T \leq T_\ell \quad k_0 = \frac{C_s}{C_\ell}$$

- Scheil model: complete mixing of solute in liquid and no mixing of solute in solid is assumed

$$f_s = 1 - \left(\frac{T_m - T}{T_m - T_\ell} \right)^{\frac{1}{k_0-1}}; \quad T_s \leq T \leq T_\ell$$

Phase change kinetics

- Solution of temperature, concentration and velocity field on macro level by a meshless method
- The phase change can be achieved by undercooling a liquid below its melting temperature
- Equilibrium melting temperature:

$$T_f = T_m + m \left(\langle C_\ell \rangle^\ell - C_0 \right) - \Gamma \kappa$$

- The interface growth velocity:

$$V_g^* (\mathbf{p}, t) = \mu_k \left(T_f - T (\mathbf{p}, t) \right) + V_v (\mathbf{v}); \quad \mathbf{p} = \Gamma_{s,\ell}$$

- Grain growth as a function of velocity, assuming no back diffusion in the solid (Wang and Beckermann, 1996a.):

$$V_v (\mathbf{v}) = \frac{4\sigma^* D_\ell m_\ell (k_0 - 1) C_\ell^*}{\Gamma} \text{Pe}_t^2; \quad C_\ell^* = \frac{T - T_m}{m_\ell}; \quad \Omega = \frac{C_\ell^* - \langle C_\ell \rangle^\ell}{C_\ell^* (1 - k_0)}$$

Phase change kinetics

- For computational efficiency, the inverse of the analytical solution has been curve fitted
- Diffusion-dominated growth:

$$\text{Pe}_t = a \left(\frac{\Omega}{1-\Omega} \right)^b ; a = 0.4567; b = 1.195$$

- Convection-dominated growth:

$$\text{Pe}_t = a \left(\frac{\Omega}{1-\Omega} \right)^b ; \text{Pe}_\infty = \left| \langle \mathbf{v}_\ell \rangle^\ell - \langle \mathbf{v}_s \rangle^s \right| R_t / D_\ell$$
$$a = 0.4567 + 0.173 \text{Pe}_\infty^{0.55} ; b = 1.195 - 0.145 \text{Pe}_\infty^{0.16}$$

Phase change kinetics

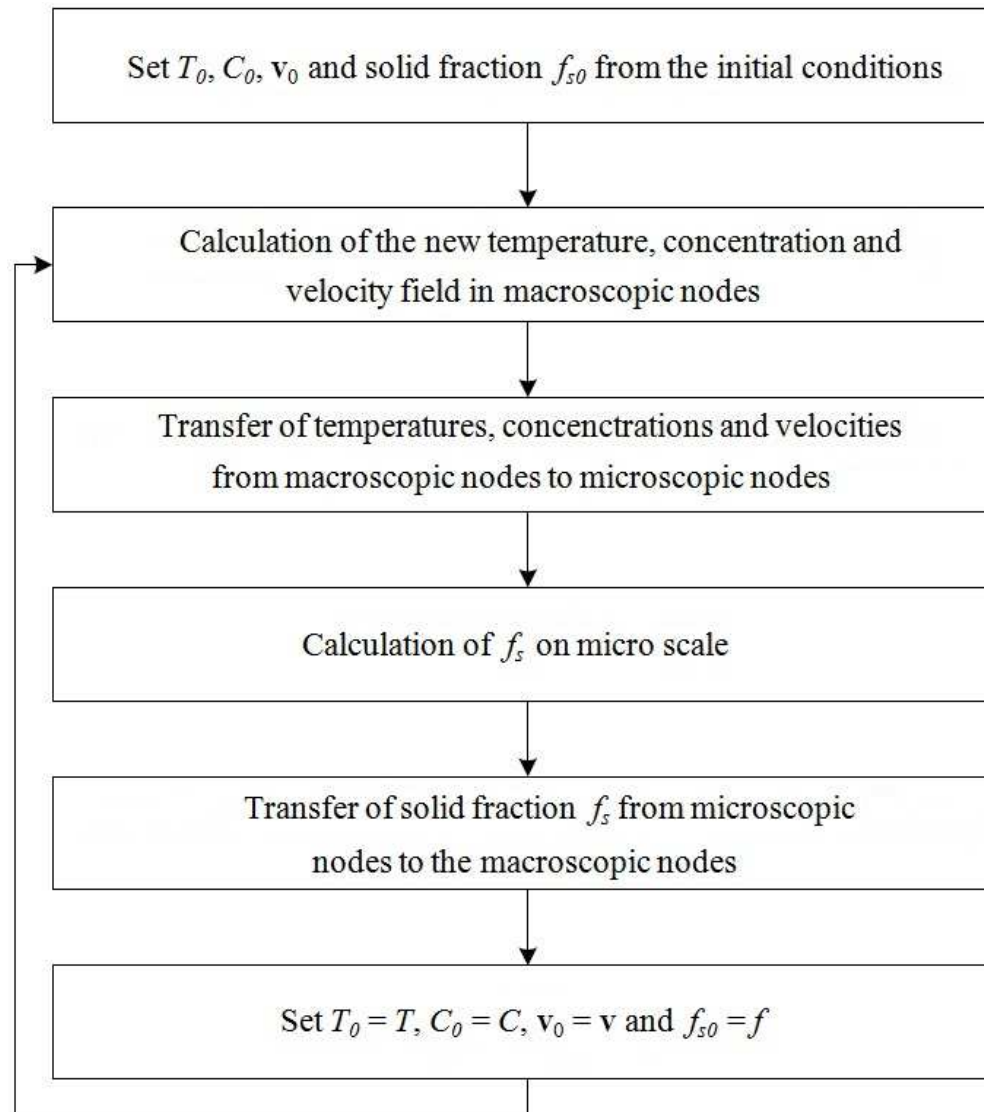
- Thermodynamic anisotropy:

$$\Gamma = \bar{\Gamma} \left[1 - \delta_t \cos \left(S \left(\theta - \theta_{def} \right) \right) \right]$$

- Kinetic anisotropy:

$$V = V_g^* (\mathbf{p}, t) \left[1 - \delta_k \cos \left(S \left(\theta - \theta_{def} \right) \right) \right]$$

Coupling of micro and macro equations



Computational model

- The transport equations for each phase are averaged separately and then summed up by taking into account the interphase balances

Macro scale equations:

$$\mathcal{R} = \begin{cases} 1 & g_s > g_s^c \\ 0 & g_s \leq g_s^c \end{cases}$$

$$\mathbf{v} = f_\ell \mathbf{v}_\ell + f_s \mathbf{v}_s$$

$$\rho = g_\ell \rho_\ell + g_s \rho_s$$

$$g_k = \frac{\rho}{\rho_k} f_k$$

$$f_s + f_\ell = 1; \quad g_s + g_\ell = 1$$

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \frac{\rho}{f_\ell} (\nabla \mathbf{v}) \mathbf{v} = -f_\ell \nabla p + \mu \nabla^2 \mathbf{v} - \mathcal{R} \left(f_\ell \frac{\mu}{K} \mathbf{v} \right)$$

$$-(1 - \mathcal{R}) \nabla \cdot (\rho f_s f_\ell \mathbf{v}_r \mathbf{v}_r) + f_\ell \mathbf{b}$$

$$\rho \frac{\partial h}{\partial t} + \rho \mathbf{v} \cdot \nabla h = \lambda \nabla^2 T$$

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C_\ell = 0$$

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{v}_s n) = \dot{N}$$

$$\mathbf{v}_r = \frac{2(\rho_s - \rho_\ell)}{9 \mu_\ell} \mathbf{g} d^2$$

$$K = K_0 \frac{f_\ell^3}{(1 - f_\ell)^2}$$

$$\mathbf{b} = \rho_{\text{ref}} [1 - \beta_T (T - T_{\text{ref}}) - \beta_C (C_\ell - C_{\text{ref}})] \mathbf{g}$$

$$h = c_p T + f_\ell L$$

$$\dot{N} = \begin{cases} N_0 \delta(t) & \text{if } T < T_{\text{nucl}} \text{ and } \int_0^t \dot{N}^\Phi dt = 0 \\ N_0 \delta(t) & \text{if } T < T_{\text{nucl}} \text{ and } N = 0 \\ 0 & \text{else} \end{cases}$$

Computational model

- The transport equations for each phase are averaged separately and then summed up by taking into account the interphase balances

Micro scale equations:

$$T_f = T_m + m_\ell (C_\ell - C_0) - \Gamma \kappa$$

$$V_g^*(\mathbf{p}, t) = \mu_k (T_f - T(\mathbf{p}, t)) + V_v(\mathbf{v}); \quad \mathbf{p} = \Gamma_{s,\ell}$$

$$V_v(\mathbf{v}) = \frac{4\sigma^* D_\ell m_\ell (k_0 - 1) C_\ell^*}{\Gamma} \text{Pe}_t^2$$

$$C_\ell^* = \frac{T - T_m}{m_\ell}$$

$$\Omega = \frac{C_\ell^* - \langle C_\ell \rangle^\ell}{C_\ell^* (1 - k_0)}$$

$$\Gamma = \bar{\Gamma} \left[1 - \delta_t \cos(S(\theta - \theta_{def})) \right]$$

$$V = V_g^*(\mathbf{p}, t) \left[1 - \delta_k \cos(S(\theta - \theta_{def})) \right]$$

Computational model

- The initial and boundary conditions:

$$\mathbf{v}(x=W, t) = \mathbf{v}(y=H, t) = \mathbf{v}(y=0, t) = 0$$

$$\frac{\partial}{\partial x} \mathbf{v}_y(x=0, t) = 0$$

$$\frac{\partial}{\partial x} T(x=W, t) = \frac{q}{\lambda} (T - T_{ext})$$

$$\frac{\partial}{\partial x} T(x=0, t) = \frac{\partial}{\partial y} T(y=0, t) = \frac{\partial}{\partial y} T(y=H, t) = 0$$

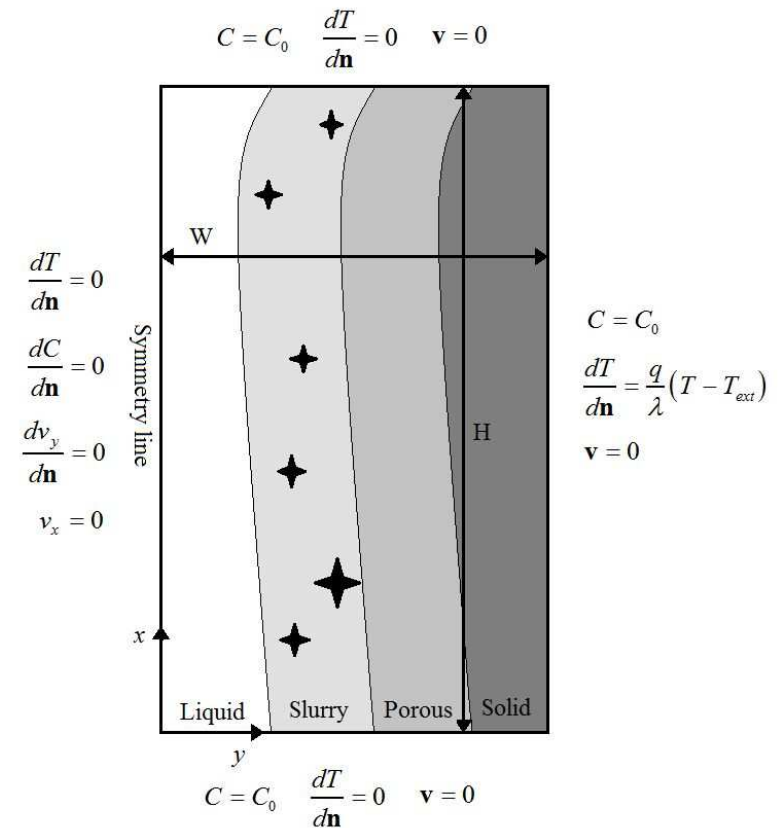
$$\frac{\partial}{\partial x} C(x=0, t) = 0$$

$$C(x=W, t) = C(y=H, t) = C(y=0, t) = C_0$$

$$\mathbf{v}(\mathbf{p}, t=0) = 0$$

$$T(\mathbf{p}, t=0) = T_0$$

$$C(\mathbf{p}, t=0) = C_0$$



Computational model

- Comparison between the models (governing equations):

$$\mathcal{R} = \begin{cases} 1 & g_s > g_s^c \\ 0 & g_s \leq g_s^c \end{cases}$$

$$\mathbf{v} = g_\ell \mathbf{v}_\ell + g_s \mathbf{v}_s$$

$$\mathbf{v} = g_\ell \mathbf{v}_\ell$$

- Mass balance:

$$\nabla \cdot \mathbf{v} = 0$$

$$\nabla \cdot \mathbf{v} = 0$$

- Momentum balance:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho g_\ell \mathbf{v}) + \nabla \cdot (\rho g_\ell \mathbf{v} \mathbf{v}) &= -g_\ell \nabla p + g_\ell \mu_\ell \nabla^2 \mathbf{v} \\ -\mathcal{R} \left(\frac{g_\ell^2 \mu_\ell}{K} \mathbf{v} \right) - (1 - \mathcal{R}) \nabla \cdot (\rho g_s g_\ell \mathbf{v}_r \mathbf{v}_r) &+ g_\ell \tilde{\rho} \mathbf{g}, \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho g_\ell \mathbf{v}) + \nabla \cdot (\rho g_\ell \mathbf{v} \mathbf{v}) &= \\ -g_\ell \nabla p + g_\ell \mu_\ell \nabla^2 \mathbf{v} - \frac{g_\ell^2 \mu_\ell}{K} \mathbf{v} &+ g_\ell \tilde{\rho} \mathbf{g}, \end{aligned}$$

- Energy balance:

$$\rho \frac{\partial h}{\partial t} + \rho \mathbf{v} \cdot \nabla h = \lambda \nabla^2 T$$

$$\rho \frac{\partial h}{\partial t} + \rho \mathbf{v} \cdot \nabla h = \lambda \nabla^2 T$$

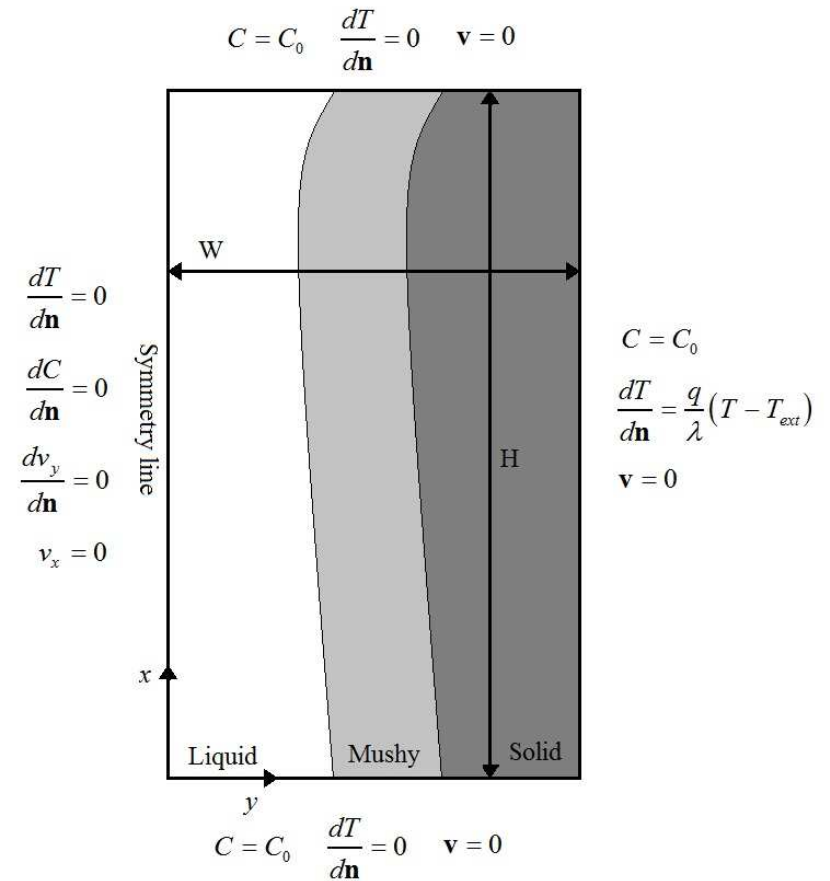
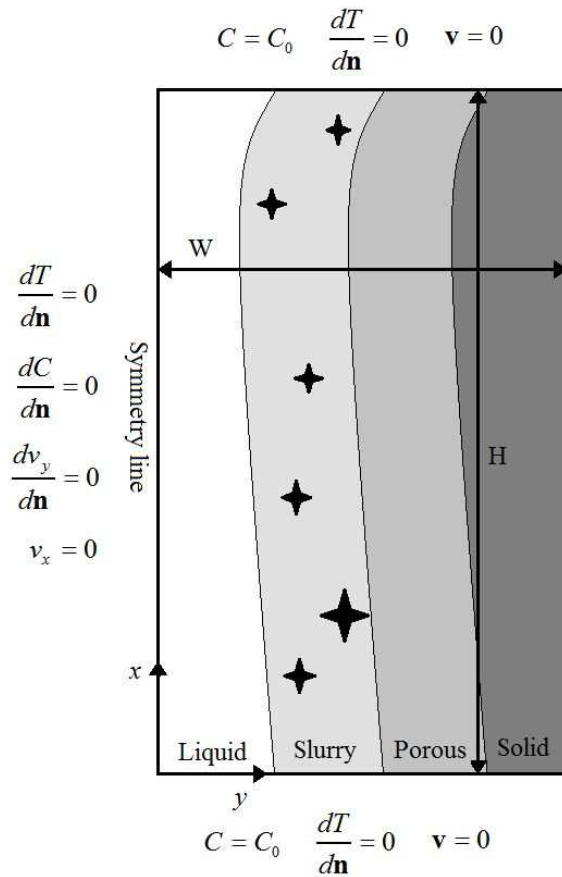
- Species balance:

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C_\ell = 0$$

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C_\ell = 0$$

Computational model

- Comparison between the models:





Conclusions

- Introduction to physical phenomena in solidification
- Overview of physical modelling of solidification systems on the macroscopic and microscopic scale
- Description of point automata method
- Developed coupling of microscopic and macroscopic equations

Future steps:

- Solving the solidification system with movement of the solid phase by LRBFCM
 - Temperatures,
 - Concentrations,
 - Velocities,
 - Pressure,
 - Grain structure, size and concentration
- Comparison with measurements (Fautrelle, Grenoble)

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THANK YOU FOR YOUR ATTENTION!