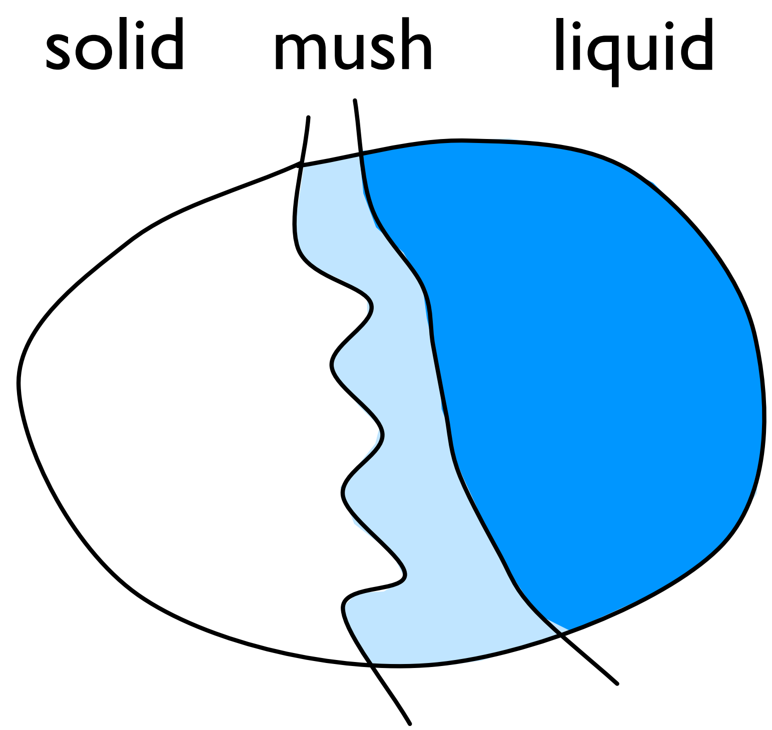


Enthalpy Method

Introduction

M.S Darwish

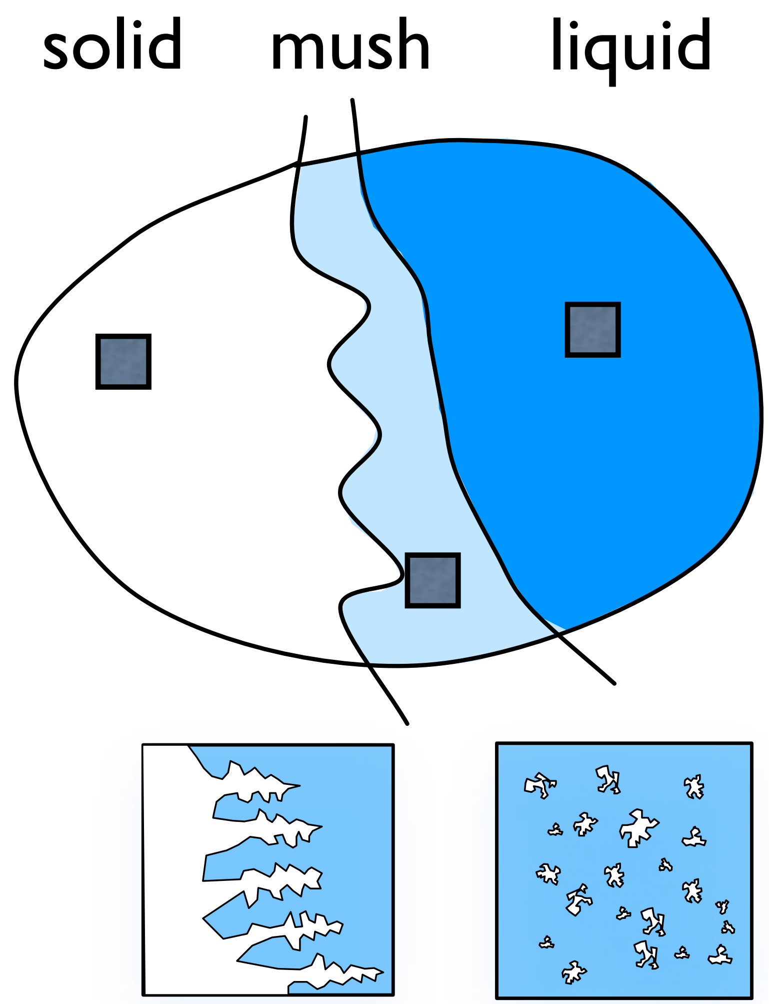
MECH 636: Solidification Modelling

The Mushy Zone

Conservation of Energy

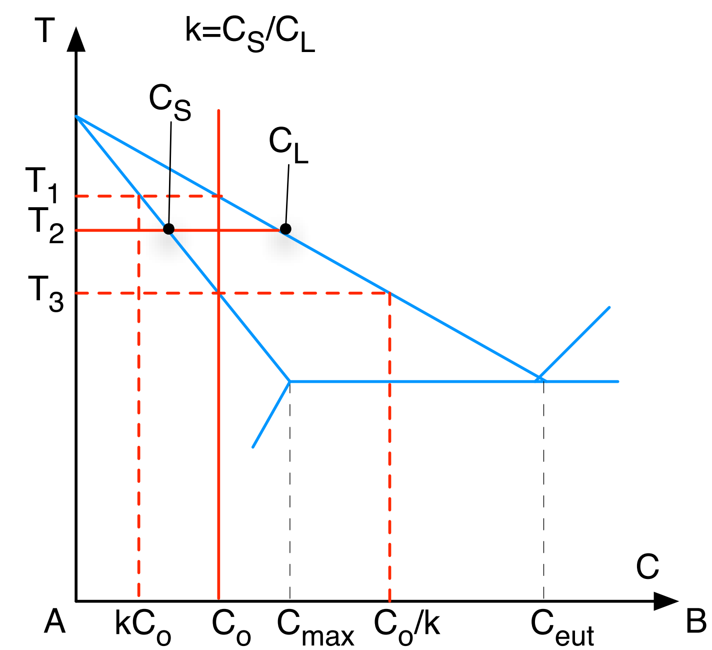
$$\frac{\partial(\rho^s h^s)}{\partial t} = \nabla \cdot (k^s \nabla T) + (Interface\ term)^s$$

$$h^s = \int_{Tref}^{T} c^s dT$$



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

$$h^l = \int_{Tref}^{T} c^l dT + L$$

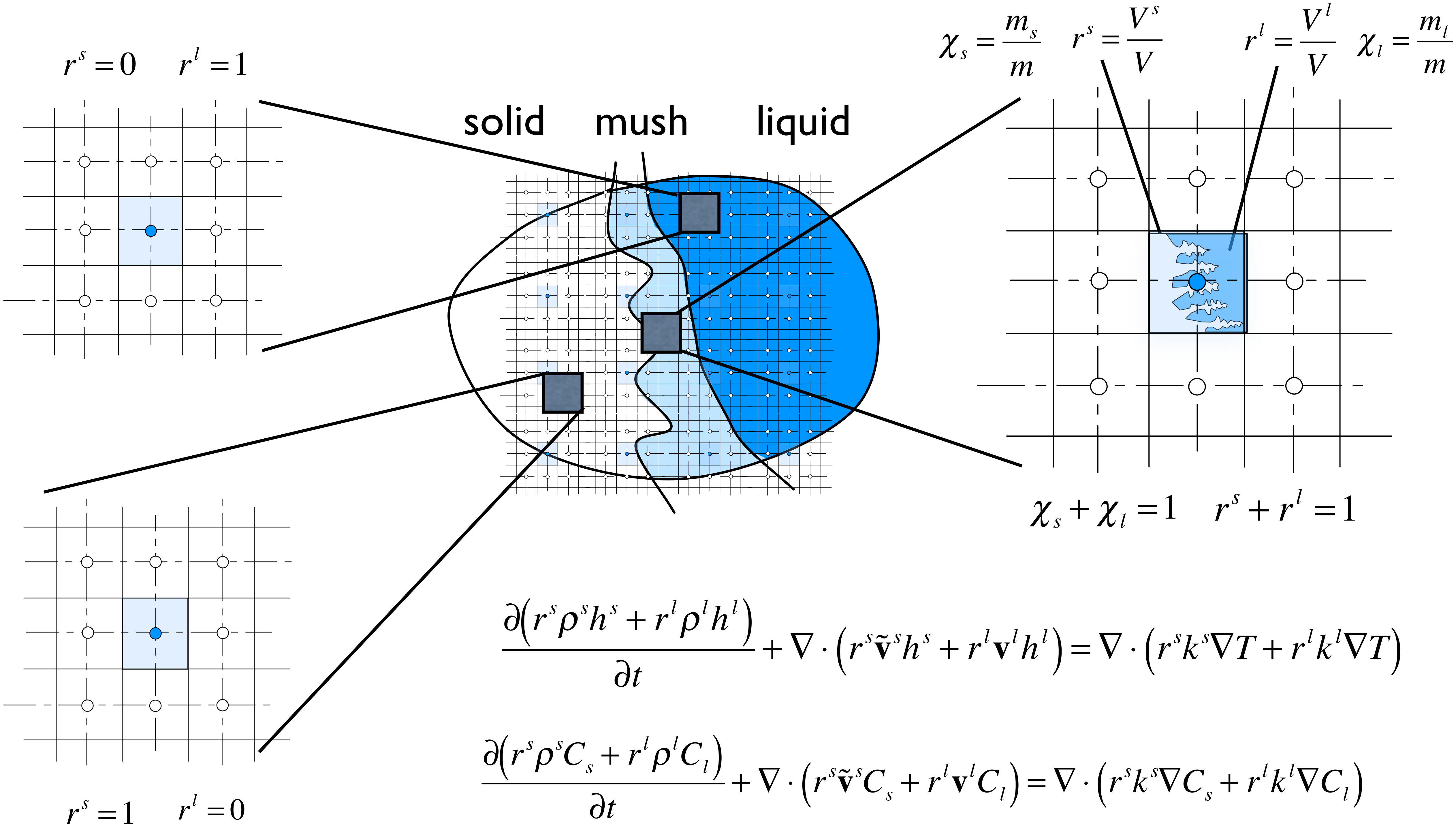


Conservation of Specie

$$\frac{\partial(\rho^s C_s)}{\partial t} = \nabla \cdot (D^s \nabla C_s)$$

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

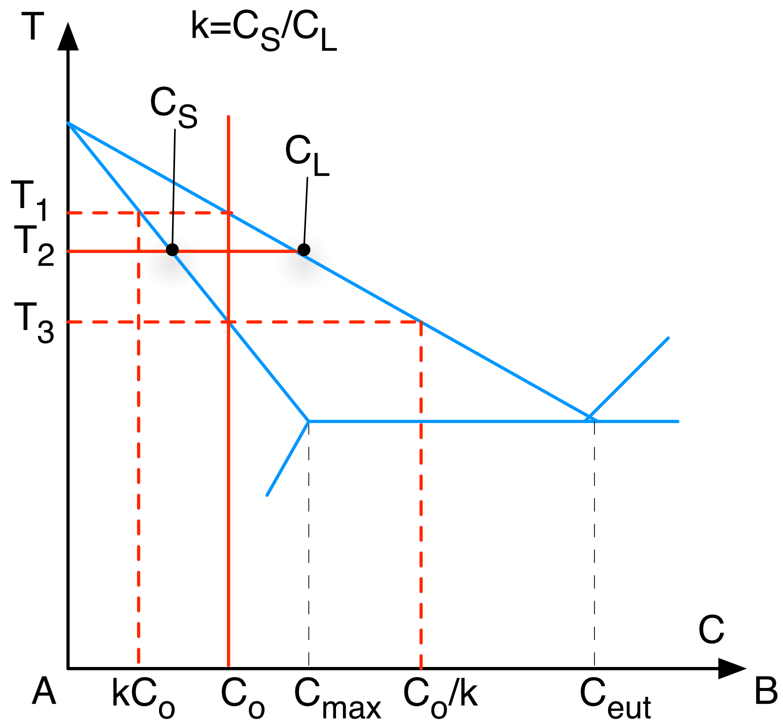
Averaging



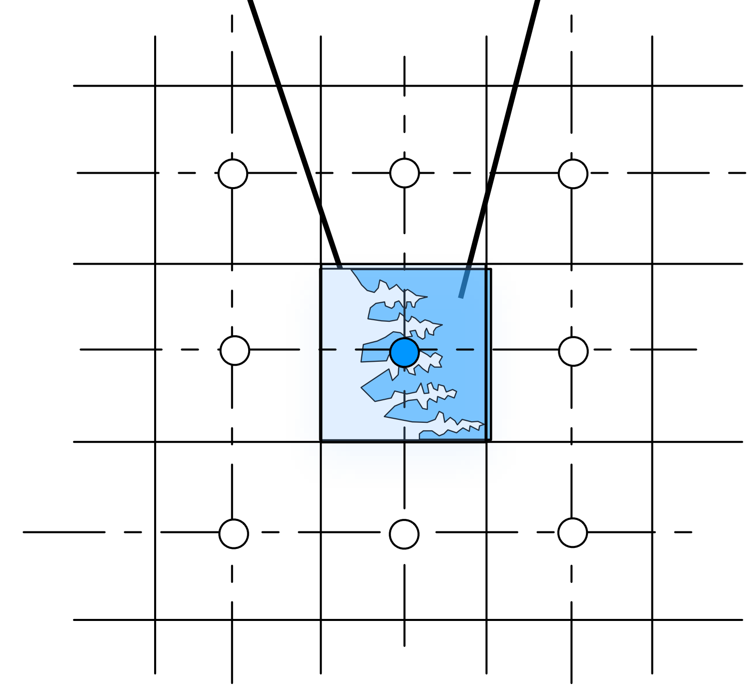
$$\frac{\partial\left(r^s\rho^s h^s + r^l\rho^l h^l\right)}{\partial t} + \nabla\cdot\left(r^s\tilde{\mathbf{v}}^s h^s + r^l\mathbf{v}^l h^l\right) = \nabla\cdot\left(r^s k^s\nabla T + r^l k^l\nabla T\right)$$

$$\frac{\partial\left(r^s\rho^s C_s + r^l\rho^l C_l\right)}{\partial t} + \nabla\cdot\left(r^s\tilde{\mathbf{v}}^s C_s + r^l\mathbf{v}^l C_l\right) = \nabla\cdot\left(r^s k^s\nabla C_s + r^l k^l\nabla C_l\right)$$

Mass and Volume Fractions



$$\chi_s = \frac{m_s}{m} \quad r^s = \frac{V^s}{V} \quad r^l = \frac{V^l}{V} \quad \chi_l = \frac{m_l}{m}$$



$$\chi_s + \chi_l = 1 \quad r^s + r^l = 1$$

mass fraction

$$\chi_s = \frac{C_l - C_o}{C_l - C_s} = \frac{m_s}{m}$$

volume fraction

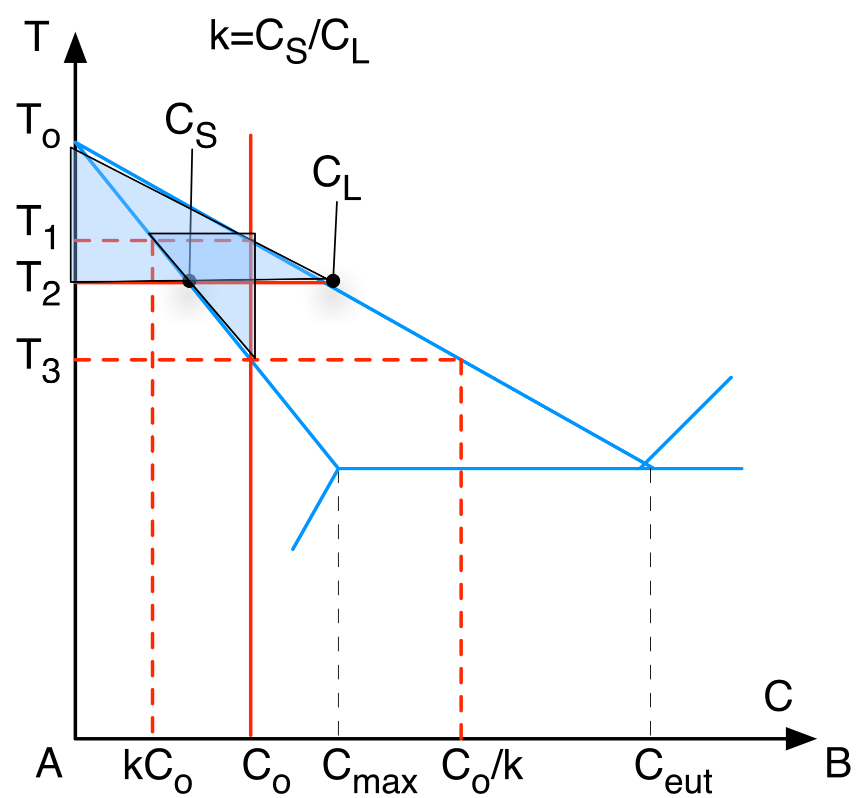
$$r_s = \frac{V_s}{V}$$

$$\frac{\chi_s}{r^s} = \frac{m_s}{m} \times \frac{V}{V_s} = \frac{\rho_s}{\rho}$$

$$r_s = \chi_s \frac{\rho}{\rho_s} = \frac{C_l - C_o}{C_l - C_s} \frac{\rho}{\rho_s}$$

$$r_l = \chi_l \frac{\rho}{\rho_l} = \frac{C_o - C_s}{C_l - C_s} \frac{\rho}{\rho_l}$$

Equilibrium Relations



$$\frac{C_l}{C_o} = \frac{T_1 - T_2}{T_0 - T_2} \qquad \frac{C_o - C_s}{C_o - kC_o} = \frac{T_2 - T_3}{T_1 - T_3} \qquad \chi_s = \frac{C_l - C_o}{C_l - C_s} = \frac{m_s}{m}$$

$$C_l = C_o \frac{T_0 - T_2}{T_0 - T_1} \qquad C_s = C_o\left(1 - (1-k)\frac{T_2 - T_3}{T_1 - T_3}\right) \qquad \chi_s = \frac{T_1 - T_2}{(1-k)(T_0 - T_2)}$$

$$r_s = \frac{T_1 - T_2}{(1-k)(T_0 - T_2)}\left(\frac{\rho}{\rho_s}\right)$$

Average Energy Equations

$$T_{ref} = 0$$

$$\frac{\partial(r_s\rho_s h_s + r_l\rho_l h_l)}{\partial t} + \nabla\cdot(r_s\rho_s\tilde{\mathbf{v}}_s h_s + r_l\rho_l\mathbf{v}_l h_l) = \nabla\cdot(r_s k_s\nabla T + r_l k_l\nabla T)$$

1

$$r_s\rho_s h_s + r_l\rho_l h_l = r_s\rho_s\int_{Tref}^{T} c_{p,s}dT + r_l\rho_l\left(\int_{Tref}^{T} c_{p,l}dT + \delta H\right)$$

$$= \rho_m\int_{Tref}^{T} c_{p,s}dT + r_l\rho_l\delta H$$

mixture

$$h_l = \int_{Tref}^{T} c_{p,l}dT + L$$

$$= \int_{Tref}^{T} c_{p,s}dT + \delta H$$

$$\delta H = \int_{Tref}^{T}(c_{p,l} - c_{p,s})dT + L$$

2

$$r_s\rho_s\tilde{\mathbf{v}}_s h_s + r_l\rho_l\mathbf{v}_l h_l = r_s\rho_s\tilde{\mathbf{v}}_s\int_{Tref}^{T} C_s dT + r_l\rho_l\mathbf{v}_l\left(\int_{Tref}^{T} C_s dT + \delta H\right)$$

$$= r_m\rho_m\mathbf{v}_m\int_{Tref}^{T} C_s dT + r_l\rho_l\mathbf{v}_l\delta H$$

mixture

$$\rho_m = r_s\rho_s + r_l\rho_l$$

$$\mathbf{v}_m = \frac{r_s\rho_s\tilde{\mathbf{v}}_s + r_l\rho_l\mathbf{v}_l}{r_m\rho_m}$$

3

$$r_s k_s\nabla T + r_l k_l\nabla T = k_m\nabla T$$

mixture

$$k_m = r_s k_s + r_l k_l$$

Assumptions

$$\int_{Tref}^{T} C\,dT \approx C \int_{Tref}^{T} dT$$

$$T_{ref} = 0$$

$$\frac{\partial\left(\rho_m c_{p,s} T + r_l \rho_l \delta H\right)}{\partial t} + \nabla \cdot \left(\rho_m \mathbf{v}_m T + r_l \rho_l \mathbf{v}_l L\right) = \nabla \cdot \left(k_m \nabla T\right)$$

Neglecting Convection

$$\frac{\partial\left(\rho_m c_{p,s} T\right)}{\partial t} = \nabla \cdot \left(k_m \nabla T\right) - \frac{\partial\left(r_l \rho_l \delta H\right)}{\partial t}$$

Discretizing

old

old

$$\frac{\rho_m c_{p,s} T_P V_P - \rho_m^{\bullet} c_{p,s}^{\bullet} T_P^{\bullet}}{\Delta t} = \sum_{f=nb(P)} \left(k_m \nabla T \cdot d\mathbf{S}\right)_f - \frac{r_l \rho_l \delta H_P - r_l^{\bullet} \rho_l^{\bullet} \delta H_P^{\bullet}}{\Delta t}$$

Algebraic Form

$$a_P T_P = \sum_{NB(P)} a_{NB} T_{NB} + b_P + a_P^t T_P^{\bullet} - \frac{V \rho_l \delta H}{\Delta t}\left(r_{l,P} - r_{l,P}^{\bullet}\right)$$

Average Specie Equation

$$\boxed{\frac{\partial(r_s\rho_s C_s + r_l\rho_l C_l)}{\partial t}} + \boxed{\nabla\cdot(r_s\rho_s\tilde{\mathbf{v}}_s C_s + r_l\rho_l\mathbf{v}_l C_l)} = \boxed{\nabla\cdot(r_s D_s\nabla C_s + r_l D_l\nabla C_l)}$$

1

$$r_s\rho_s C_s + r_l\rho_l C_l = \rho_m C_m$$

mixture

$$C_m = \frac{r_s\rho_s C_s + r_l\rho_l C_l}{\rho_m}$$

2

$$r_s\rho_s\tilde{\mathbf{v}}_s C_s + r_l\rho_l\mathbf{v}_l C_l \;= (r_s\rho_s\tilde{\mathbf{v}}_s k + r_l\rho_l\mathbf{v}_l)C_l \;= \rho_m\mathbf{v}_m C_l$$

mixture

$$\mathbf{v}_m = \frac{r_s\rho_s\tilde{\mathbf{v}}_s k + r_l\rho_l\mathbf{v}_l}{\rho_m}$$

3

$$r_s D_s\nabla C_s + r_l D_l\nabla C_l \;= r_s D_s\nabla(kC_l) + r_l D_l\nabla C_l \;= D_m\nabla C_l$$

mixture

$$D_m = r_s k D_s + r_l D_l$$

$$\frac{\partial(\rho_m C_m)}{\partial t} + \nabla \cdot (\rho_m \mathbf{v}_m C_l) = \nabla \cdot (D_m \nabla C_l)$$

$$C_m = \chi_s C_s + \chi_l C_l \quad = \frac{m_s}{m} C_s + \frac{m_l}{m} C_l \quad \Leftrightarrow mC_m = m_s C_s + m_l C_l$$

$$\frac{m}{V} C_m = \frac{m_s}{V} C_s + \frac{m_l}{V} C_l$$

$$\rho_m C_m = \frac{m_s}{V} \frac{V_s}{V_s} C_s + \frac{m_l}{V} \frac{V_l}{V_l} C_l$$

$$\rho_m C_m = r_s \rho_s C_s + r_l \rho_l C_l$$

$$= r_s \rho_s k C_l + r_l \rho_l C_l$$

$$= \rho_m C_l - r_s \rho_s (1-k) C_l$$

$$\frac{\partial(\rho_m C_l)}{\partial t} + \nabla \cdot (\rho_m \mathbf{v}_m C_l) = \nabla \cdot (D_m \nabla C_l) + \frac{\partial\left(r_s \rho_s (1-k) C_l\right)}{\partial t}$$

$$\boxed{\frac{\partial(\rho_m C_l)}{\partial t} = \nabla \cdot (D_m \nabla C_l) + \frac{\partial\left(r_s \rho_s (1-k) C_l\right)}{\partial t}}$$

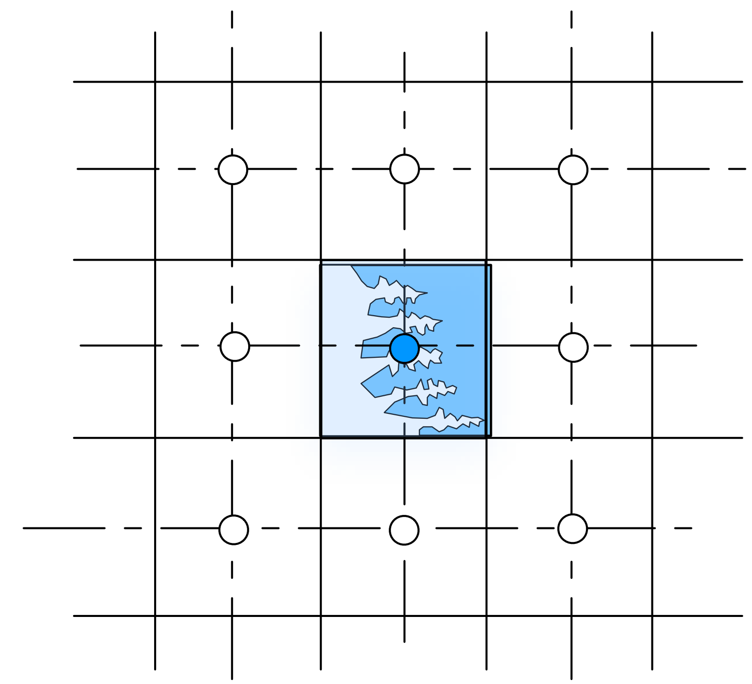
Case 1: no Specie diffusion

$$\frac{\partial(\rho_m C_m)}{\partial t} = 0$$

$$\frac{\partial(\rho_m c_{p,s} T)}{\partial t} = \nabla \cdot (k_m \nabla T) - \frac{\partial(r_l \rho_l \delta H)}{\partial t}$$

$$a_P T_P = \sum_{NB(P)} a_{NB} T_{NB} + b_P + a_P^t T_P^{\bullet} - \frac{V \rho_l \delta H}{\Delta t}\left(r_{l,P} - r_{l,P}^{\bullet}\right)$$

$$r_l = f(T) = \begin{cases} 1 & T > T_{Liquidus} \\ \dfrac{T - T_{Liquidus}}{T_{Liquidus} - T_{solidus}} & T_{solidus} < T < T_{Liquidus} \\ 0 & T < T_{solidus} \end{cases}$$



$\chi_s + \chi_l = 1$ $\quad r^s + r^l = 1$

Liquid Fraction Update

$$a_P T_P = \sum_{NB(P)} a_{NB} T_{NB} + b_P + a_P^t T_P^{\bullet} + \frac{V\rho_l \delta H}{\Delta t}\left(r_{l,P} - r_{l,P}^{\bullet}\right)$$

$$T_P = f^{-1}(r_{l.P})$$

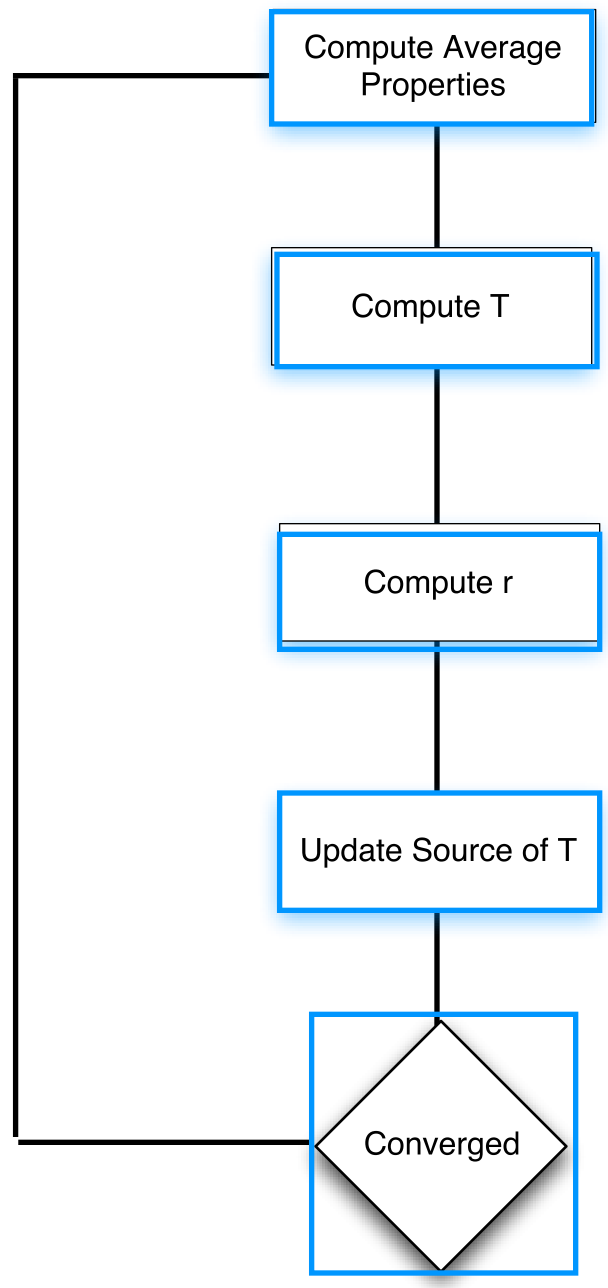
$$a_P f^{-1}(r_{l.P}) = \sum_{NB(P)} a_{NB} T_{NB} + b_P + a_P^t T_P^{\bullet} - \frac{V\rho_l \delta H}{\Delta t}\left(r_{l,P} + \delta r_{l,P} - r_{l,P}^{\bullet}\right)$$

$$\delta r_{l,P} = a_P \Delta t \frac{T_P - f^{-1}(r_{l.P})}{V\rho_l \delta H}$$

$$r_{l,P}^{n+1} = r_{l,P}^{n} + \delta r_{l,P}$$

$$0 \le r_{l,P}^{n+1} \le 1$$

Algorithm


Compute Average Properties
Compute T
Compute r
Update Source of T
Converged

case 2: Specie Diffusion

$$\frac{\partial\left(\overline{\rho}\overline{C}\right)}{\partial t}+\nabla\cdot\left(r^s\tilde{\mathbf{v}}^sC_s+r^l\mathbf{v}^lC_l\right)=\nabla\cdot\left(r^sD^s\nabla C_s+r^lD^l\nabla C_l\right)$$

Under equilibrium conditions a discontinuity exist at the solid/liquid interface given by

$$C_l=C_s/k$$

$$C=\chi_lC_l+\chi_sC_s$$

$$\chi_l=\frac{m_l}{m}$$

$$mC=m_lC_l+m_sC_s$$

$$\rho VC=\rho_lV_lC_l+\rho_sV_sC_s$$

$$\rho C=\rho_l\frac{V_l}{V}C_l+\rho_s\frac{V_s}{V}C_s$$

$$=\rho_lr_lC_l+\rho_sr_skC_l$$

$$=(\rho-\rho_sr_s)C_l+\rho_sr_skC_l$$

$$=\rho C_l-(1-k)\rho_sr_sC_l$$

$$\rho C=\rho C_l-(1-k)\rho_sr_sC_l$$

$$\chi_l=\frac{m_l}{m}=\frac{\rho_lV_l}{\rho V}=r_l\frac{\rho_l}{\rho}$$

$$\chi_l=\frac{C_o-C_s}{C_l-C_s}$$

$$\rho=\rho_lr_l+\rho_sr_s$$

$$\rho=\rho_l\frac{V_l}{V}+\rho_s\frac{V_s}{V}$$

$$\frac{\partial\left(\overline{\rho}\overline{C}\right)}{\partial t}+\nabla\cdot\left(r^s\tilde{\mathbf{v}}^sC_s+r^l\mathbf{v}^lC_l\right)=\nabla\cdot\left(r^sD^s\nabla C_s+r^lD^l\nabla C_l\right)$$

$$\rho V=\rho_lV_l+\rho_sV_s$$

$$\frac{\partial\left(\overline{\rho}\overline{C}\right)}{\partial t}+\nabla\cdot\left(r^{s}\tilde{\mathbf{v}}^{s}C_{s}+r^{l}\mathbf{v}^{l}C_{l}\right)=\nabla\cdot\left(r^{s}D^{s}\nabla C_{s}+r^{l}D^{l}\nabla C_{l}\right)$$

$$r^{s}D^{s}\nabla C_{s}+r^{l}D^{l}\nabla C_{l}=\left(r^{s}D^{s}+r^{l}D^{l}k\right)\nabla C_{l}\quad=\overline{D}^{*}\nabla C_{l}$$

$$\frac{\partial\left(\overline{\rho}C_{l}\right)}{\partial t}+\nabla\cdot\left(\overline{\rho}\mathbf{v}^{*}C_{l}\right)=\nabla\cdot\left(\overline{D}^{*}\nabla C_{l}\right)$$

Algorithm

Unknowns

T

r_l, r_s

χ_l, χ_s

C, C_l, C_s

Equations Conservation of Energy (T)

Relations