Numerical method for 1D simulation using enthalpy method

Joseph Fishlock

May 23, 2023

Contents

1 Non-Dimensional Equations

There are two models (non-dimensional systems of conservation equations to be solved). We work in non-dimensional variables in 1D (z, t). For non-dimensionalisation see Page 6. We use the lagrangian derivative in a moving frame with velocity V.

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + V\frac{\partial f}{\partial z}. \tag{1.1}$$

The three primary non-dimensional variables bulk enthalpy ($\mathscr{H}_l$), bulk salinity (Θ) and bulk gas (Γ) are governed by conservation equations. All other variables are obtained by an equilibrium enthalpy method calculation. The liquid Darcy velocity (W_l) is obtained in the full model by conservation of mass (elliptic pressure equation). In the reduced model it is free to be imposed as a forcing from a brine convection model. In both models gas Darcy velocity is calculated as

$$W_g = \phi_g V_g = \phi_g \left(\frac{\mathscr{B}}{K(\lambda)} + 2G(\lambda)\frac{W_l}{\phi_l}\right), \tag{1.2}$$

where λ is the ratio of bubble size to tube size. If we assume a scaling for tube size of the form $R_T = R_0\phi_l^q$, then $\lambda = R_B/R_0\phi_l^q$. $K(\lambda)$ and $G(\lambda)$ are empirical functions for a spherical centered bubble in Stokes flow in a cylinder.

1.1 Full model

We retain the conservation of total volume ($\phi_s + \phi_l + \phi_g = 1$). This implies changing gas fraction drives liquid flow. Full model conservation equations

$$\frac{D\mathscr{H}}{Dt} = -\frac{\partial}{\partial z}\left[\mathscr{H}_l W_l\right] + \frac{\partial^2\theta}{\partial z^2}, \tag{1.3}$$

$$\frac{D\Theta}{Dt} = -\frac{\partial}{\partial z}\left[W_l(\Theta_l + \mathscr{C})\right] + \frac{1}{\mathrm{Le}_S}\frac{\partial}{\partial z}\left[\phi_l\frac{\partial\Theta_l}{\partial z}\right], \tag{1.4}$$

$$\frac{D\Gamma}{Dt} = -\frac{\partial}{\partial z}\left[W_l\chi\omega)\right] - \frac{\partial W_g}{\partial z} + \frac{\chi}{\mathrm{Le}_\xi}\frac{\partial}{\partial z}\left[\phi_l\frac{\partial\omega}{\partial z}\right], \tag{1.5}$$

$$\frac{D\phi_g}{Dt} = \frac{\partial}{\partial z}\left[-\Pi(\phi_l)\frac{\partial p}{\partial z}\right]. \tag{1.6}$$

Note: $W_l = -\Pi\frac{\partial p}{\partial z}$.

1.2 Reduced model

We neglect the gas fraction so that $\phi_s + \phi_l = 1$. The conservation equations remain the same Eqs. (1.3) to (1.5). We no longer need to solve for pressure as no flow is driven. The calculation of the enthalpy method is significantly easier as gas fraction is decoupled from thermal solve. We can reconstruct approximations to the full phase fractions ϕ^* as follows. In solid region assume $\phi_l^* = \phi_l = 0$, $\phi_g^* = \phi_g$ and $\phi_s^* = 1 - \phi_g$. In other regions $\phi_s^* = \phi_s$, $\phi_g^* = \phi_g$ and $\phi_l^* = 1 - \phi_s - \phi_g$. This means we must impose the extra constraint that prevents more gas accumulating in a region that would already be saturated. This is done in the numerics by setting $V_g = 0$ if the cell above is such that $\phi_g \geq 1 - \phi_s$.

2 Enthalpy method

From the primary variables ($\mathscr{H}$, Θ, Γ) we seek to reconstruct the other state variables: temperature (θ), liquid salinity (Θ_l), solid salinity (Θ_s), solid fraction (ϕ_s), liquid fraction (ϕ_l), gas fraction (ϕ_g), and dissolved gas concentration (ω).

This is done using the following phase plane information in each region:

- liquid ($\mathscr{H} > \mathscr{H}_L$): $\phi_s = 0$ and solid salinity undetermined so set $\Theta_s = -\mathscr{C}$.
- mush ($\mathscr{H}_E < \mathscr{H} \leq \mathscr{H}_L$): liquidus $\theta = \theta_L(\Theta_l) = -\Theta_l$, and fresh ice $\Theta_s = -\mathscr{C}$.
- eutectic ($\mathscr{H}_S < \mathscr{H} \leq \mathscr{H}_E$): $\theta = -1$, $\Theta_l = 1$.
- solid ($\mathscr{H} \leq \mathscr{H}_S$): $\phi_l = 0$, liquid salinity undetermined so set $\Theta_l = 1$.

The phase boundaries are determined for each region by applying the conditions in both.
The gas saturation state depends on $\Gamma_{\text{sat}} = \chi\phi_l$.

- Super saturated ($\Gamma \geq \Gamma_{\text{sat}}$): saturation $\omega = 1$ and $\phi_g = \Gamma - \Gamma_{\text{sat}}$.
- Sub saturated ($\Gamma < \Gamma_{\text{sat}}$): $\phi_g = 0$ and $\omega = \Gamma/\Gamma_{\text{sat}}$.

2.1 Full enthalpy method

For the full enthalpy method calculation we use the relations:

$$\phi_s + \phi_l + \phi_g = 1, \tag{2.1}$$

$$\mathscr{H} = \theta(1-\phi_g) - \phi_s \mathrm{St}, \tag{2.2}$$

enthalpy in each phase is $\mathscr{H}_l = \theta$, $\mathscr{H}_s = \theta - \mathrm{St}$ and $\mathscr{H}_g = 0$

$$\Theta = \phi_s\Theta_s + \phi_l\Theta_l - \phi_g\mathscr{C}, \tag{2.3}$$

$$\Gamma = \chi\omega\phi_l + \phi_g. \tag{2.4}$$

This is tricky as everything is fully coupled and the enthalpy phase boundaries depend on both salinity and gas content. See Page 15 for derivation.

2.2 Reduced enthalpy method

assuming $\phi_s + \phi_l = 1$ for the enthalpy and salt is extremely useful as it reduces to usual enthalpy method [1]:

$$\phi_s + \phi_l = 1, \tag{2.5}$$

$$\mathscr{H} = \theta - \phi_s \mathrm{St}, \tag{2.6}$$

$$\Theta = \phi_s\Theta_s + \phi_l\Theta_l. \tag{2.7}$$

The gas variables can then be solved independent of phase later using only Γ and $\phi_l(\mathscr{H}, \Theta)$. This yields the following expressions.

$$\mathscr{H}_L = -\Theta, \tag{2.8}$$

$$\mathscr{H}_E = \frac{\mathrm{St}}{1+\mathscr{C}}(\Theta - 1) - 1, \tag{2.9}$$

$$\mathscr{H}_S = -1 - \mathrm{St}. \tag{2.10}$$

2.2.1 liquid

$$\phi_s = 0,$$

$$\phi_l = 1,$$

$$\theta = \mathscr{H},$$

$$\Theta_l = \Theta,$$

$$\Theta_s = -\mathscr{C}.$$

2.2.2 mush

$$\phi_l = 1 - \phi_s,$$

$$\Theta_s = -\mathscr{C},$$

$$\Theta_l = -\theta,$$

$$\theta = \mathscr{H} + \phi_s \mathrm{St},$$

$$\phi_s = \frac{-B - \sqrt{B^2 - 4AC}}{2A},$$

where $A = \mathrm{St}$, $B = \mathscr{H} - \mathrm{St} - \mathscr{C}$, $C = -(\mathscr{H} + \Theta)$.

2.2.3 eutectic

$$\theta = -1,$$

$$\Theta_l = 1,$$

$$\phi_l = 1 - \phi_s,$$

$$\phi_s = \frac{-(1 + \mathscr{H})}{\mathrm{St}},$$

$$\Theta_s = \frac{\Theta + \phi_s - 1}{\phi_s}.$$

Note that this means that on the mush side of the eutectic we get the solid fraction $\phi_s = (1 - \Theta)/(1 + \mathscr{C})$.

2.2.4 solid

$$\phi_l = 0,$$

$$\phi_s = 1,$$

$$\Theta_l = 1,$$

$$\Theta_s = \Theta,$$

$$\theta = \mathscr{H} + \mathrm{St}.$$

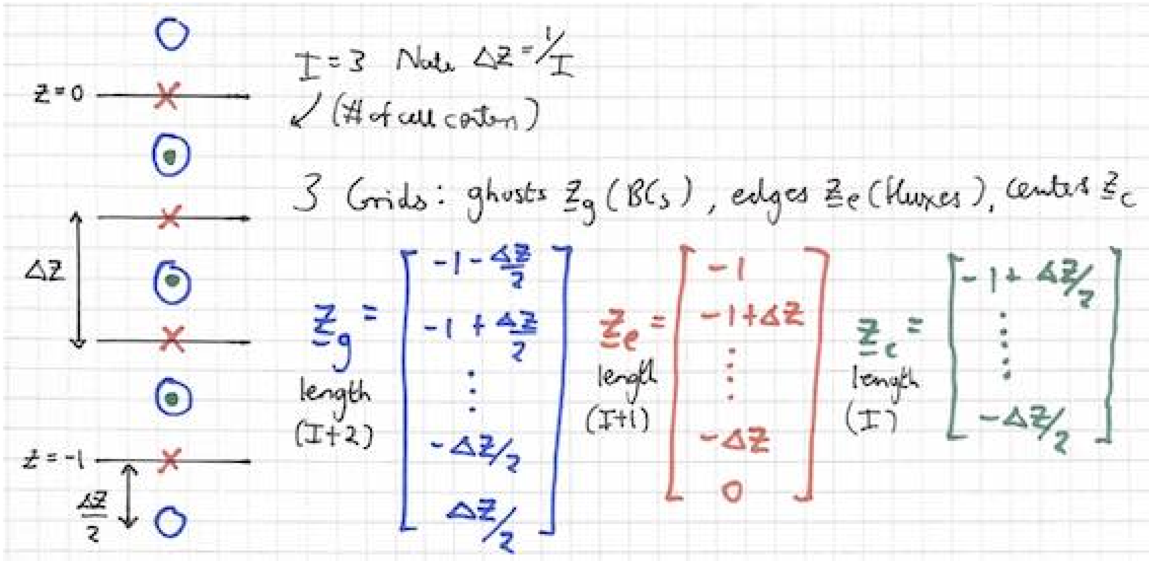


Figure 1: Diagram of three different girds quantities can sit on in spatial discretisation.

3 Spatial discretisation

We discretise the vertical spatial dimension into I cells of width $\Delta z = 1/I$. Each of these cells has a center and two edges. The cell centers lie on the centered grid $\boldsymbol{z}_c$. The cell edges lie on the edge grid $\boldsymbol{z}_e$. The cell centers plus a ghost cell for boundary conditions at the top and bottom lie on the ghost grid $\boldsymbol{z}_g$. See Fig. 1 for a diagram of the grids.

Quantities that lie on the ghost grid are written $\hat{\boldsymbol{f}} = \boldsymbol{f}(\boldsymbol{z}_g, t)$. Quantities that lie on the edge grid are written $\overline{\boldsymbol{f}} = \boldsymbol{f}(\boldsymbol{z}_e, t)$. Quantities that lie on the center grid are written $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{z}_c, t)$. Note that any quantities on the ghost grid must be given appropriate boundary conditions.

To take derivatives of a quantity on the ghost grid we multiply by the difference matrix $\boldsymbol{D_g}$. This has dimensions $(I+1, I+2)$ and returns the derivative on the edge grid. To take derivatives of a quantity on the edge grid we multiply by the difference matrix $\boldsymbol{D_e}$. This has dimensions $(I, I+1)$ and returns the derivative on the center grid. Both of these matrices are all zero apart from $-1/\Delta z$ on the leading diagonal (i, i), and $1/\Delta z$ on the first off diagonal $(i, i+1)$. Note that matrix multiplication is written $\cdot$ and two quantities on the same grid may be multiplied elementwise.

We introduce two functions for taking ghost grid quantities to edge grid quantities. First the upwinding function $\mathscr{U}$(ghost, edge). This takes a quantity on the ghost grid and a flux on the edge grid and returns their product, where the ghost value is chosen to be the cell on the side of the edge where the velocity is coming from. Second the geometric mean function $\mathscr{G}$(ghost). This interpolates a quantity on the ghost grid to the edge grid by taking the geometric average of the two neighbouring cell centers. This is useful as if one of the two cells has no liquid then the edge will have none which makes it impermeable.

We write the spatially discretised equations as

$$\frac{\partial \boldsymbol{H}}{\partial t} = -\boldsymbol{D_e} \cdot \overline{\boldsymbol{F}_{\mathscr{H}}}, \tag{3.1}$$

$$\frac{\partial \boldsymbol{\Theta}}{\partial t} = -\boldsymbol{D_e} \cdot \overline{\boldsymbol{F}_{\Theta}}, \tag{3.2}$$

$$\frac{\partial \boldsymbol{\Gamma}}{\partial t} = -\boldsymbol{D_e} \cdot \overline{\boldsymbol{F}_{\Gamma}}, \tag{3.3}$$

where the fluxes are given by

$$\overline{\boldsymbol{F}_{\mathscr{H}}} = \mathscr{U}(\hat{\boldsymbol{\mathscr{H}}}, \overline{\boldsymbol{V}}) + \mathscr{U}(\hat{\boldsymbol{\mathscr{H}}}_l, \overline{\boldsymbol{W}_l}) - \boldsymbol{D_g} \cdot \hat{\boldsymbol{\theta}}, \tag{3.4}$$

$$\overline{\boldsymbol{F}_{\Theta}} = \mathscr{U}(\hat{\boldsymbol{\Theta}}, \overline{\boldsymbol{V}}) + \mathscr{U}(\hat{\boldsymbol{\Theta}}_l + \mathscr{C}, \overline{\boldsymbol{W}_l}) - \frac{1}{\mathrm{Le}_S} \mathscr{G}(\hat{\boldsymbol{\phi}}_l) \boldsymbol{D_g} \cdot \hat{\boldsymbol{\Theta}}_l, \tag{3.5}$$

$$\overline{\boldsymbol{F}_{\Gamma}} = \mathscr{U}(\hat{\boldsymbol{\Gamma}}, \overline{\boldsymbol{V}}) + \mathscr{U}(\chi \hat{\boldsymbol{\omega}}, \overline{\boldsymbol{W}_l}) + \mathscr{U}(\hat{\boldsymbol{\phi}_g}, \overline{\boldsymbol{V}_g}) - \frac{\chi}{\mathrm{Le}_\xi} \mathscr{G}(\hat{\boldsymbol{\phi}}_l) \boldsymbol{D_g} \cdot \hat{\boldsymbol{\omega}}. \tag{3.6}$$

These fluxes give the finite volume first order upwind scheme in space.

The pressure (if used) is given by solving the following linear system

$$\boldsymbol{M} \cdot \hat{\boldsymbol{p}} = \frac{\partial \hat{\boldsymbol{\phi}_g}}{\partial t} + \boldsymbol{D_e} \cdot \mathscr{U}(\hat{\boldsymbol{\phi}_g}, \overline{V}), \tag{3.7}$$

where the matrix is given by $\boldsymbol{M} = \boldsymbol{D_e} \cdot \boldsymbol{K} \cdot \boldsymbol{D_g}$. Where $\boldsymbol{K}$ is the diagonal matrix of size $(I+1, I+1)$ formed by $-\overline{\boldsymbol{\Pi}}$. To prevent the system becoming singular it is necessary to add a small numerical regularisation to this matrix. This prevents the permeability ever being actually zero. Boundary conditions are added to the matrix $\boldsymbol{M}$ and forcing term to give $W_l = 0$ at $z = 0$ and $p = 0$ at $z = -1$.

4 Solvers

4.1 lagged solver for full model

This solver, chosen as "LU", solves the full model. You specify a constant timestep. The pressure equation Eq. (3.7) requires information about the gas fraction at the current and future timestep. Therefore we take a forward euler timestep of the conservation equations e.g:

$$\mathscr{H}^{n+1} = \mathscr{H}^{n} - \Delta t \boldsymbol{D}_e \cdot \overline{\boldsymbol{F}_{\mathscr{H}}}^{n}. \tag{4.1}$$

This step gives a value of the gas fraction at both the current and next timestep which is then used to solve for W_l. In this way the liquid velocity is always lagged one timestep behind the other quantities.

4.2 Reduced solver forward euler

This solver, chosen as "RED", solves the reduced model using forward euler for a fixed timestep. It is exactly the same as the lagged solver (see Section 4.1), but without the extra complication of solving for the liquid velocity and the enthalpy method is much simpler.

4.3 Scipy solver

This solver, chosen as "SCI", solves the reduced model using the same finite volume upwind scheme. However, the temporal discretisation is handled entirely by the scipy function solve ivp in the integration module. This comes with a number of benefits as it handles adaptive timestepping well so long as we specify the max timestep should be small enough to satisfy the stability of explicit treatment of the thermal diffusion term i.e. $\Delta t < \Delta z^2/2$.

5 Non-dimensionalisation

Dimensional Equations

2023/05/11

Assume:

* $\rho_l = \rho_s = \rho$ = constant
* ρ_g constant

$$\frac{D\phi_g}{Dt} = \nabla \cdot \underline{u}_l$$

$H_s = \rho c_p (T - T_i) - \rho L$

$$\frac{DH}{Dt} + \nabla \cdot (H_l \underline{u}_l) = \nabla \cdot (\bar{k} \nabla T)$$

$H = \phi_s H_s + \phi_l H_l$, $H_l = \rho c_p (T - T_i)$

$$\frac{DS}{Dt} + \nabla \cdot (S_l \underline{u}_l) = \nabla \cdot (\phi_l D_s \nabla S_l)$$

$S = \phi_s S_s + \phi_l S_l$ as mass ratio

bulk salinity

$$\frac{DG}{Dt} + \nabla \cdot (\rho_l \xi_l \underline{u}_l) + \nabla \cdot (\rho_g \underline{u}_g) = \nabla \cdot (\rho_l \phi_l D_g \nabla \xi_l)$$

$G = \rho_l \phi_l \xi_l + \rho_g \phi_g$

bulk gas mass per unit volume

$$W_g = \phi_g \left(\frac{V_{stokes}}{K_1(\lambda)} + \frac{2 G(\lambda)}{\phi_l} W_l \right)$$

vertical only

$\underline{u}_l = W_l \hat{\underline{z}}$, $\underline{u}_g = W_g \hat{\underline{z}}$

$\lambda = R_B / R_T$, $R_T \sim R_0 \phi_l^{\,q}$

Conservation of Water

2023/05/11

Liquid phase contains : H_2O, Salt (aq), Gas(aq)

mass ratio $S_\ell = \frac{\text{kg of salt}}{\text{kg of liquid}}$ density of liquid phase ρ_ℓ (in principle a function of composition)

mass ratios : $\underset{\text{wat.}}{W_\ell} + \underset{\text{salt}}{S_\ell} + \underset{\text{gas}}{\xi_\ell} = 1$

By analogy solid phase contains : $H_2O(s)$, Salt (s)

$W_s + S_s = 1$

W_s: $\frac{\text{kg ice}}{\text{kg of solid}}$ S_s: $\frac{\text{kg of salt}}{\text{kg of solid}}$

Total mass of H_2O in system per volume $= \rho_\ell \phi_\ell W_\ell + \rho_s \phi_s W_s$

Can be advected in liquid phase

$$\Rightarrow \frac{D}{Dt}(\rho_\ell \phi_\ell W_\ell + \rho_s \phi_s W_s) + \nabla \cdot (\rho_\ell W_\ell \underset{\text{liq Darcy vel}}{\underline{u}_\ell}) = 0$$

Assumptions :

- $W_\ell \approx 1$, $W_s \approx 1$
- $\rho_\ell = \rho_s = \rho =$ constant

$\Downarrow$

$$\frac{D\phi_g}{Dt} = \nabla \cdot \underline{u}_\ell$$

* Assume gas volume change doesn't drive much flow (i.e $\phi_g \ll 1$) $\Rightarrow \nabla \cdot \underline{u}_\ell = 0$

2023/05/11

Conservation of Heat

Enthalpy per unit volume H

$H_s = \rho_s C_{p,s}(T-T_i) - \rho_s L$

$H_\ell = \rho_\ell C_{p,\ell}(T-T_i)$

T_i is reference temperature

latent heat of fusion

at $T=T_i$: $\frac{H_s}{\rho_s} - \frac{H_\ell}{\rho_\ell} = -L$

Specific heat capacity C_p s.t. $\left.\frac{\partial H}{\partial T}\right|_{\text{fixed phase}} = \rho C_p$.

* Neglect enthalpy in gas phase as $\rho_g \ll \rho_\ell, \rho_s$

$\Rightarrow$ total enthalpy per unit vol $= H = \phi_s H_s + \phi_\ell H_\ell = (\rho_s\phi_s C_{p,s} + \rho_\ell\phi_\ell C_{p,\ell})(T-T_i) - \rho_s\phi_s L$.

$(+H_0)$ set enthalpy of liquid at $T=T_i$ to $H_0 = 0$.

Enthalpy can be advected in liquid or conducted:

$$\frac{DH}{Dt} + \nabla\cdot(H_\ell \underline{u}_\ell) = \nabla\cdot(\bar{k}\nabla T)$$

thermal conductivity: $\bar{k} = \phi_\ell k_\ell + \phi_s k_s + \phi_g k_g$ (typically $k_g \ll k_\ell, k_s$).

Can use $\frac{D\phi_g}{Dt} = \nabla\cdot\underline{u}_\ell$

& $C_{p,g} = k_g = 0$, $C_{p,s} = C_{p,\ell} = C_p$, $\rho_s = \rho_\ell = \rho$

$\Rightarrow$

$$\rho C_p(1-\phi_g)\frac{DT}{Dt} + \rho C_p \underline{u}_\ell\cdot\nabla T = \rho L\frac{D\phi_s}{Dt} + \nabla\cdot(k(1-\phi_g)\nabla T)$$

Can allow insulating effect of air even if we approximate $\phi_s + \phi_\ell \simeq 1$ everywhere else as $k_g = 0$

$$\frac{DH}{Dt} + \nabla\cdot(H_\ell \underline{u}_\ell) = \nabla\cdot(k(1-\phi_g)\nabla T)$$

Assume: $C_{p,s} = C_{p,\ell} = C_p$

$\rho_s = \rho_\ell = \rho$

$k_s = k_\ell = k$

$\phi_s + \phi_\ell = 1$ (i.e. $\phi_g \ll 1$)

$\kappa = \frac{k}{\rho C_p}$

$$\rho C_p\frac{DT}{Dt} + \rho C_p \underline{u}_\ell\cdot\nabla T = \rho L\frac{D\phi_s}{Dt} + k\nabla^2 T$$

2023/05/11

Conservation of Salt

$$\frac{D}{Dt}\left(\rho_\ell \phi_\ell S_\ell + \rho_s \phi_s S_s\right) + \nabla\cdot\left(\rho_\ell S_\ell \underline{u}_\ell\right) = \nabla\cdot\left(\rho_\ell \phi_\ell D_s \nabla S_\ell\right)$$

total mass of salt per unit volume

advection in liquid

molecular diffusion in liquid

Conservation of Gas

gas Darcy vel

$$\frac{D}{Dt}\left(\rho_\ell \phi_\ell \xi_\ell + \rho_g \phi_g\right) + \nabla\cdot\left(\rho_\ell \xi_\ell \underline{u}_\ell\right) + \nabla\cdot\left(\rho_g \underline{u}_g\right) = \nabla\cdot\left(\rho_\ell \phi_\ell D_\xi \nabla \xi_\ell\right)$$

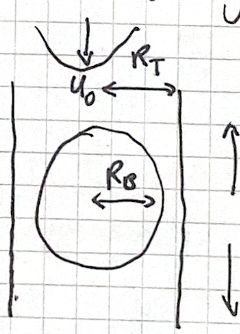
advection by bubbles

Gas Darcy Velocity

* Assume Background Liquid Darcy flow $\underline{u}_\ell$ is given by brine drainage or imposed

* Vertical direction $\underline{u}_g = W_g \hat{\underline{z}}$

Force balance bubble in tube



Buoyancy

$\underline{u}_\ell = W_\ell \hat{\underline{z}}$

drag from liquid flow

drag from walls

$$\Rightarrow V_g = \frac{V_{stokes}}{K_1(\lambda)} + G(\lambda)\, U_0$$

interstitial bubble velocity.

maximum interstitial liquid velocity in Poiseuille profile

$$V_{stokes} = \frac{\Delta\rho g R_B^2}{3\mu_\ell}$$

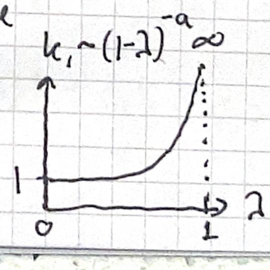
$$U_0 = \frac{2W_\ell}{\phi_\ell}$$

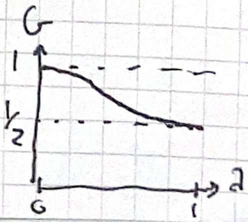
$$\lambda = \frac{R_B}{R_T} \Rightarrow \lambda(R_B, \phi_\ell)$$

$$R_T \sim R_0 \phi_\ell^{q} \quad \text{(Experimental)}$$

$\Delta\rho \simeq \rho_\ell$ $\quad W_g = V_g \phi_g$

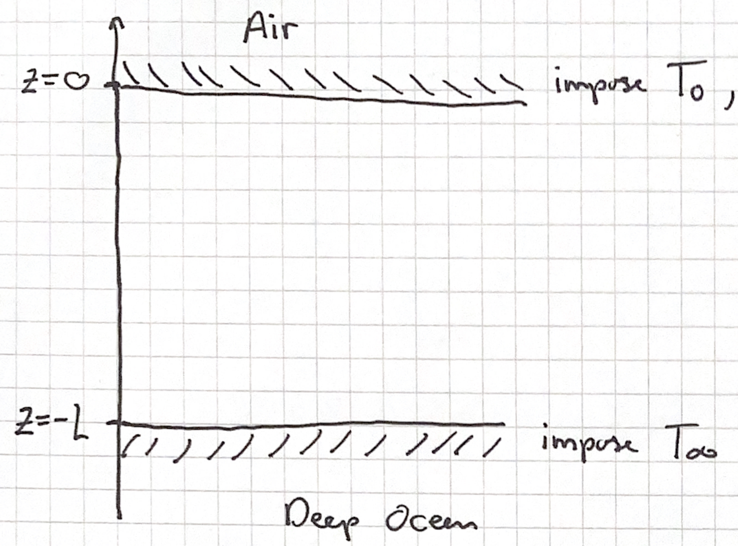
$$W_g = \phi_g \left(\frac{\rho_\ell g R_B^2}{3\mu K_1(\lambda)} + \frac{2G(\lambda)}{\phi_\ell} W_\ell\right)$$





Scales in 1D Problem

2023/05/11



thermal diffusivity $\kappa = \frac{K}{\rho c_p}$ (conductivity; spec heat capacity)

moving frame V

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} - V\frac{\partial f}{\partial z}.$$

S_i is Ocean salinity $\approx 35 g/kg$

domain depth L

Lengths $z \sim L$ **Time** $t \sim L^2/\kappa$ (thermal diffusion) **Velocity** $V, W_\ell, W_g \sim \kappa/L$ (scale of thermal diffusive growth)

Salt differences $\Theta = \frac{S - S_i}{\Delta S}$ (relative to ocean water scaled by typical variation).

$\Delta S = S_E - S_i$ ($230 g/kg$)

$\Theta = 0$ ocean water $\quad \mathcal{C} = \frac{S_i}{\Delta S}$.

$\Theta = -\mathcal{C}$ fresh

Temperature differences $\theta = \frac{T - T_i}{T_i - T_E}$ (relative to ocean freezing temperature).

$\Delta T = T_i - T_E$

$T_i = T_L(S_i)$ liquidus freezing temp of ocean water.

Dissolved gas $\omega = \frac{\xi_\ell}{\xi_{sat}}$ (relative to saturation concentration).

Bulk gas $\Gamma = \frac{G}{\rho_g}$ (gas density)

Enthalpy $H \sim \rho c_p \Delta T$ (from temp scale)

$\Rightarrow \mathcal{H}_\ell = \frac{H_\ell}{\rho c_p \Delta T} = \theta \qquad \mathcal{H}_s = \frac{H_s}{\rho c_p \Delta T} = \theta - \frac{L}{\rho c_p}$ (Stefan number)

Bulk enthalpy: $\mathcal{H} = \frac{H}{\rho c_p \Delta T} = \phi_s \mathcal{H}_s + \phi_\ell \mathcal{H}_\ell = \phi_s(\theta - St) + \phi_\ell \theta = (1-\phi_g)\theta - \phi_s St$

Bulk salt: $\Theta = \frac{S - S_i}{\Delta S} = \frac{\phi_s(S_s - S_i)}{\Delta S} + \frac{\phi_\ell(S_\ell - S_i)}{\Delta S} - \frac{\phi_g S_i}{\Delta S} = \phi_s\Theta_s + \phi_\ell\Theta_\ell - \phi_g \mathcal{C}$

neglect $\phi_g \ll 1$ for reduced

Bulk gas: $\Gamma = \frac{G}{\rho_g} = \left(\frac{\rho_\ell \xi_{sat}}{\rho_g}\right)\omega\phi_\ell + \phi_g = \chi\omega\phi_\ell + \phi_g$

1D Non Dimensional Equations

2023/05/13

$$\frac{D\phi_g}{Dt} = \frac{\partial W_l}{\partial z}$$

$$\lambda = \frac{R_B}{R_T} = \frac{R_B}{R_0 \phi_l^q} = \frac{\Lambda}{\phi_l^q}$$

$$W_g = \phi_g\left(\frac{\mathcal{B}}{K_1(\lambda)} + \frac{2G(\lambda)}{\phi_l} W_l\right)$$

Liner liquidus $T_L(S_l) = T_i + \Gamma_L(S_i - S_l)$

s.t $\Delta T = \Gamma_L \Delta S$

$\Rightarrow \theta_L(\Theta_l) = -\Theta_l$

Solidus (no segregation coeff)

$\Theta_s = -1$

$$\frac{DH}{Dt} + \frac{\partial}{\partial z}(H_l W_l) = \frac{\partial^2 \theta}{\partial z^2}$$

$k_s = k_l = k_g$

$\rightarrow$ if $k_s = k_l$, $k_g = 0$ then $\frac{\partial}{\partial z}\left((1-\phi_g)\frac{\partial \theta}{\partial z}\right)$

$H = (1-\phi_g)\theta - \phi_s St$ $\quad H_l = \theta$

$$\frac{D\Theta}{Dt} + \frac{\partial}{\partial z}((\Theta_l + C_e)W_l) = \frac{1}{Le_s}\frac{\partial}{\partial z}\left(\phi_l \frac{\partial \Theta_l}{\partial z}\right)$$

$\Theta = \phi_s \Theta_s + \phi_l \Theta_l - \phi_g C_e$

$$\frac{D\Gamma}{Dt} + \frac{\partial}{\partial z}(\chi \omega W_l) + \frac{\partial W_g}{\partial z} = \frac{\chi}{Le_\xi}\frac{\partial}{\partial z}\left(\phi_l \frac{\partial \omega}{\partial z}\right)$$

$\Gamma = \chi \omega \phi_l + \phi_g$

Non-Dimensional Numbers

2023/05/13

$$St = \frac{L}{c_p \Delta T} \qquad \mathcal{C} = \frac{S_i}{\Delta S} \qquad Le_S = \frac{D_S}{\kappa} \qquad Le_\xi = \frac{D_\xi}{\kappa}$$

$$\chi = \frac{\rho_\ell \xi_{sat}}{\rho_g} \qquad \mathcal{B} = \frac{V_{st}}{V} = \frac{\rho_\ell g R_B^2 L}{3\mu\kappa} \qquad \lambda = \frac{R_B}{R_0}$$

We also have non-dimensional BCs:

$z=0$ (top):

cold temp: $\theta_0(t)$

No salt flux or fixed salinity θ_0

Fixed gas e.g $\Gamma_0 = \Gamma_{sat}(\mathcal{H}_0, \theta_0)$

$z=-1$ (ocean):

$\theta(z=-1) = \theta_\infty$

Ocean salinity $\Theta(z=-1)=0$

$\Gamma(z=-1) = \chi$

Reduced Model (makes enthalpy method much more tractable).

2023/05/13

* When gas doesn't move ϕ_g is controlled by freezing, for saturated liquid χ is the maximum volume of gas that can be exsolved

Approximation $\chi \ll 1 \Rightarrow$ neglect terms of $O(\phi_g)$ except in gas equation

$$\mathcal{H} = \Theta - \phi_s St \qquad \text{and } \phi_s + \phi_\ell = 1.$$

$$\Theta = \phi_s \Theta_s + \phi_\ell \Theta_\ell \qquad \therefore \frac{\partial W_\ell}{\partial z} \simeq 0 \text{ (no flow driven by gas)}$$

$$\Gamma = \chi \phi_\ell \omega + \phi_g$$

other conservation equations stay the same.

* This can breakdown if large gas volume accumulates below impermeable layer or gas velocity becomes much larger than liquid velocity.

* For consistency impose extra condition that ϕ_g is no larger than void fraction

Approximate scheme: (No gas fronts)

Solid : $\phi_s = 1$, $\phi_\ell = 0$

other phases (mush/liquid) : $\phi_s + \phi_\ell = 1$

In reality

$\phi_s = 1 - \phi_g$, $\phi_\ell = 0$ (the same)

ϕ_s the same

$\phi_\ell = 1 - \phi_s - \phi_g$

$\therefore \phi_g \leq \text{void frac} = 1 - \phi_s$

(so that $\phi_\ell \geq 0$)

This stops arbitrary gas accumulating in one cell and gives Boundary Layer.

* This approximation lets us evaluate Γ given $\mathcal{H}, \Theta, W_\ell$ as input.

6 Full enthalpy method derivation

Enthalpy Method With $\phi_s + \phi_l + \phi_g = 1$.

Bulk temperature T, Salinity S

$S = \phi_s S_s + \phi_l S_l$ as $S_g = 0$.

Linearised phase boundaries

$$T_L(S) = T_E - \Gamma(S_l - S_E) \quad (1)$$

$$T_S(S) = \max\left(T_E, T_E - \frac{\Gamma}{d_c}(S_s - d_c S_E)\right) \quad (2)$$

d_c distribution coeff

in mushy phase approximate $S_s = d_c S_l$.

eutectic point (T_E, S_E) s.t. $T_L(S_E) = T_S(S_E) = T_E$

fresh water freezes at $0°c$ $T_L(0) = 0 \Rightarrow T_E + \Gamma S_E = 0$

ϕ_g reduces maximum bulk salinity by occupying volume

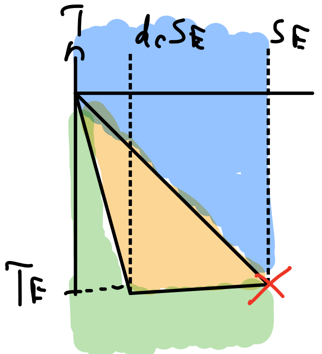
✱ Phase space for sub-eutectic Mushy Layer changes with ϕ_g

consider liquid phase $S = \phi_l S_l$ $\quad 0 \leq S_l \leq S_E$ for sub eutectic mushy layer.

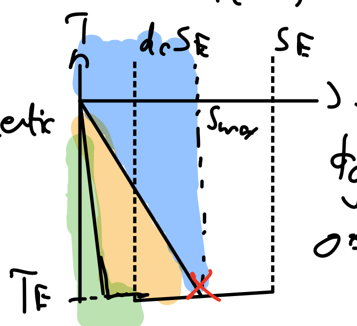
$\phi_l = 1 - \phi_g$ as $\phi_s = 0 \Rightarrow S = (1-\phi_g) S_l$

$\therefore$ $0 \leq S \leq (1-\phi_g) S_E$ so as ϕ_g increases eutectic point shifts inwards (on liquidus $\phi_s = 0, S = (1-\phi_g)S_l$ $\}$ sub into

... solidus $\phi_l = 0$, $S = (1-\phi_g)S_s$ $\}$ (1) & (2))



× = eutectic point moves as $\phi_g \uparrow$



$\phi_g = 1/2$

$0 \leq S \leq S_{max} = (1-\phi_g) S_E$

Define Bulk Quantities

(ξ_{sat} : constant otherwise going to get non linear equations for ϕ_g everywhere).

Enthalpy : $H = \phi_s H_s + \phi_l H_l + \phi_g H_g$

Salt : $S = \phi_s S_s + \phi_l S_l$

Gas : $G = \rho_l \xi_l \phi_l + \rho_g \phi_g$ $\quad G = \rho_g \Gamma$

take $\rho_l = \rho_s = \rho = \text{const}$ $\quad \varepsilon = \rho_g/\rho \ll 1$.

$\rho_g = \text{const}$

Neglect H_g term as $O(\varepsilon)$.

Take $c_{p,l} = c_{p,s}$

$H_s = \rho c_p (T - T_i) - \rho L$

$H_L = \rho c_p (T - T_i)$

$H_g = 0$.

$H = \rho c_p (T - T_i)(\phi_s + \phi_l) - \phi_s \rho L$

Note only freezing / melting changes latent heat term

gas acts as a void carrying no enthalpy

so have effective heat capacity $H = \rho c_{eff} (T - T_i) - \rho \phi_s L$

$c_{eff} = c_p(1 - \phi_g)$.

Breaks down when $\phi_g = 1$

as no energy can be retained in system.

ND.

$H = \rho c_p \Delta T \mathcal{H}$ $\quad \theta = \frac{T - T_i}{\Delta T}$ $\quad \Delta T = T_i - T_E$

$\Delta S = S_E - S_i$

$\Theta = \frac{S - S_i}{\Delta S}$ $\quad \Theta_l = \frac{S_l - S_i}{\Delta S}$, $\quad \Theta_S = \frac{S_S - S_i}{\Delta S}$.

$\mathcal{C}_e = \frac{S_i - d_c S_i}{\Delta S} = \frac{\text{difference in liquid solid salinity}}{\text{salinity variation}}$.

$\mathcal{C}_e = \frac{(1 - d_c) S_i}{\Delta S}$ $\quad 0 \leq \mathcal{C}_e \leq \infty$ $\quad St = \frac{L}{c_p \Delta T}$

$S_i \to 0$ $\quad S_i \to S_E$

$\xi_e = \xi_{sat}\, \omega$ so $\omega_{sat} = 1$. $\quad \chi = \frac{\rho \xi_{sat}}{\rho_g}$ $\quad \phi_g = O(\chi)$.

$\frac{H}{\rho c_p \Delta T} = \theta (1 - \phi_g) - \phi_S St = \mathcal{H}$ $\quad \frac{S_i}{\Delta S} = \frac{\mathcal{C}_e}{1 - d_c}$

$$\boxed{\begin{aligned} \mathcal{H}_s &= \theta - St \\ \mathcal{H}_l &= \theta . \end{aligned}}$$

$\Theta = \frac{S - S_i}{\Delta S} = \frac{\phi_S S_S + \phi_l S_l + \phi_g \times 0 - \phi_S S_i - \phi_l S_i - \phi_g S_i}{\Delta S}$

$\Theta = \phi_S \Theta_S + \phi_l \Theta_l - \phi_g \frac{S_i}{\Delta S} = \phi_S \Theta_S + \phi_l \Theta_l - \frac{\phi_g \mathcal{C}_e}{(1 - d_c)}$

So: $\quad \dfrac{-C_e}{(1-\phi_c)} \le \Theta_l \le 1$

fresh $\qquad\qquad$ eutectic

if $\phi_s = 0 \quad \Theta = (1-\phi_g)\Theta_l - \dfrac{\phi_g C_e}{(1-\phi_c)}$

$$\frac{-C_e}{(1-\phi_c)}(1-\phi_g) - \frac{\phi_g C_e}{(1-\phi_c)} = \frac{-C_e}{(1-\phi_c)} \quad \Bigg| \quad \Theta_l = 1 \quad 1 - \phi_g\left(1 + \frac{C_e}{1-\phi_c}\right)$$

So $\quad \dfrac{-C_e}{(1-\phi_c)} \le \Theta \le \Theta_{max} = 1 - \phi_g\left(1 + \dfrac{C_e}{1-\phi_c}\right)$

bulk fresh

the reduced eutectic point for a given ϕ_g $\Theta_{max}(\phi_g)$

s.t. $\Theta_{max}(0) = 1$.

note $S_{max} = (1-\phi_g)S_E$ from earlier

$$\Theta_{max} = \frac{S_{max} - S_i}{\Delta S} = \frac{(1-\phi_g)S_E - S_i}{\Delta S}$$

$$= \frac{S_E - S_i}{\Delta S} - \phi_g \frac{S_E}{\Delta S} = 1 - \phi_g\left(1 + \frac{C_e}{1-\phi_c}\right).$$

$$\frac{S_E}{\Delta S} - \frac{S_i}{\Delta S} = 1 \qquad \frac{S_E}{\Delta S} = 1 + \frac{C_e}{1-\phi_c}$$

$$\Gamma = \frac{G}{\rho_g} = \frac{\rho\, \omega\, \xi_{sat}\, \phi_\ell}{\rho_g} + \phi_g = \chi \omega \phi_\ell + \phi_g$$

SO :

$$\phi_s + \phi_l + \phi_g = 1$$

$$\mathcal{H} = \Theta(1-\phi_g) - \phi_s St$$

$$\Theta = \phi_s \Theta_s + \phi_l \Theta_\ell - \frac{\phi_g c_e}{1-d_c}$$

eutectic pont.

$$-\frac{c_e}{1-d_c} \leq \Theta \leq \Theta_{max}(\phi_g)$$

$$\Gamma = \chi \omega \phi_\ell + \phi_g$$

saturation when $\omega = 1$, $\phi_g = 0$

$\Gamma_{sat} = \chi \phi_\ell$ $\therefore$

$\Gamma \geq \Gamma_{sat}(\mathcal{H}, \Theta)$: $\omega = 1$

$\Gamma < \Gamma_{sat}(\mathcal{H}, \Theta)$: $\phi_g = 0$.

ω, ϕ_g

ϕ_s, ϕ_ℓ

$\theta, \Theta_\ell, \Theta_s$

from $\mathcal{H}, \Theta, \Gamma$.

Phases:	liquid (+ gas)	solid + liquid (+ gas)) mushy	eutectic	solid (+gas)
	$\mathcal{H} \geq \mathcal{H}_L$	$\mathcal{H}_E \leq \mathcal{H} < \mathcal{H}_L$	$\mathcal{H}_S \leq \mathcal{H} < \mathcal{H}_E$	$\mathcal{H} < \mathcal{H}_S$
	$\phi_s = 0$	$\Theta = \Theta_L(\Theta_\ell)$	$\Theta = \Theta_S(\Theta_s)$	$\phi_\ell = 0$
	Θ_s N/A	$\Theta_s = d_c \Theta_\ell - c_e$	$\Theta_\ell = 1$	Θ_ℓ N/A.

Working out ND $\left\{ \frac{S_s}{S_\ell} = d_c \ll 1 \right\}$

$S_s = d_c S_\ell$

$$\frac{\Delta S\,\Theta_s + S_i}{\Delta S\,\Theta_\ell + S_i} = d_c = \frac{\Theta_s + \frac{\mathcal{C}_e}{1-d_c}}{\Theta_\ell + \frac{\mathcal{C}_e}{1-d_c}}$$

$$d_c\left((1-d_c)\Theta_\ell + \mathcal{C}_e\right) = \Theta_S(1-d_c) + \mathcal{C}_e.$$

$$d_c(1-d_c)\Theta_\ell + d_c\mathcal{C}_e - \mathcal{C}_e = \Theta_S(1-d_c).$$

$$d_c(1-d_c)\Theta_\ell - \mathcal{C}_e(1-d_c) = \Theta_S(1-d_c)$$

$$d_c\Theta_\ell - \mathcal{C}_e = \Theta_S.$$

in Mushy phase $\mathcal{H}_E \le \mathcal{H} < \mathcal{H}_L$

$$\Theta_S = d_c\Theta_\ell - \mathcal{C}_e.$$

(as $d_c \to 0$ $\Theta_S \to -\mathcal{C}_e$).

ND Liquidus & Solidus:

so $\Delta T = \Gamma \Delta S.$

$T_L = T_E - \Gamma(S_\ell - S_E)$ $\qquad T_i = T_E - \Gamma(S_i - S_E)$

$$\Theta_L = \frac{T - T_i}{\Delta T} = \frac{T_E - T_i}{\Delta T} - \frac{\Gamma(\Delta S\,\Theta_\ell + S_i - S_E)}{\Delta T}$$

$$\Theta_L = -1 - \frac{(\Delta S\,\Theta_\ell + S_i - S_E)}{\Delta S} = -1 - (\Theta_\ell - 1)$$
$$= -1 - \Theta_\ell + 1 = -\Theta_\ell$$

$$\boxed{\theta_L(\theta_\ell) = -\theta_\ell}$$

$$T_S = \max\left(T_E, T_E - \frac{\Gamma}{d_c}(S_S - d_c S_E)\right)$$

$$\theta_S = \frac{T_S - T_i}{\Delta T} = \max\left(-1, -1 - \frac{1}{d_c \Delta S}\left(\Delta S \theta_s + S_i - d_c S_E\right)\right)$$

$$= \max\left(-1, -1 - \left(\frac{\theta_S}{d_c} + \frac{\ell_e}{d_c(1-d_c)} - \frac{S_E}{\Delta S}\right)\right)$$

$$\frac{S_E - S_i}{\Delta S} = \frac{S_E}{\Delta S} - \frac{\ell_e}{1-d_c} = 1.$$

$$\theta_S = \max\left(-1, -1 - \left(\frac{\theta_S}{d_c} + \frac{\ell_e}{d_c(1-d_c)} - 1 - \frac{\ell_e}{1-d_c}\right)\right).$$

$$\theta_S = \max\left(-1, -\frac{\theta_S}{d_c} + \frac{\ell_e}{1-d_c} - \frac{\ell_e}{d_c(1-d_c)}\right)$$

$$\theta_S = \max\left(-1, \frac{-\theta_S}{d_c} + \frac{\ell_e}{(1-d_c)d_c}(-1 + d_c)\right)$$

$$\theta_S = \max\left(-1, -\frac{\theta_S}{d_c} - \frac{\ell_e}{d_c}\right)$$

$$\boxed{\theta_S = \max\left(-1, -1/d_c(\theta_S + \ell_e)\right).}$$

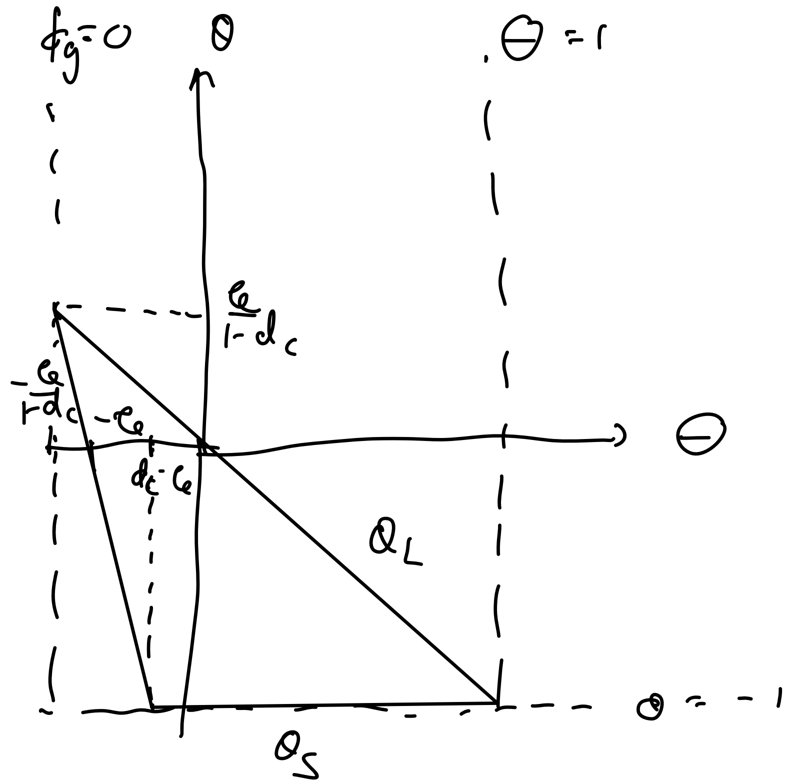
$$\theta_S = -\frac{\ell_e}{1-d_c} \quad \theta_S = \frac{\ell_e}{1-d_e}$$

$$\theta_S = -\ell_e \quad \theta_S = 0.$$

$$\theta_S = d_c - \ell_e, \; \theta_S = 1$$

$\theta_S + \ell_e = d_c \theta_\ell$ in mush

$\theta_S + \ell_e = d_c \Rightarrow \theta_\ell = 1$ in mush



Non Dimensional (T, S) phase plane at $\phi_g = 0$.

Now we calculate phase relations for $\Gamma < \Gamma_{sat}$.

so $\phi_g = 0$ and $\omega = \Gamma / \chi \phi_\ell(\mathcal{H}, \Theta)$

Liquid $(-)$:

$\phi_s = 0$, Θ_s N/A, $\phi_g = 0 \Rightarrow \phi_\ell = 1$, $\omega = \Gamma / \chi$.

Need to find θ & Θ_ℓ.

$\mathcal{H} = \theta$

$\Theta = \Theta_\ell$

Mushy phase. $\ominus$

$\theta = \theta_L = -\Theta_e \qquad \phi_g = 0 \qquad \phi_s = 1 - \phi_e$

$\Theta_s = d_c \Theta_e - C_e . \quad \omega = \Gamma / \chi \phi_e$

Need to find θ, ϕ_e

$$\mathcal{H} = \theta - (1-\phi_e) St \rightarrow 1 - \phi_e = \frac{\theta - \mathcal{H}}{St} \Rightarrow \phi_e = 1 - \frac{\theta - \mathcal{H}}{St}.$$

$$\Theta = (1-\phi_e)(-d_c\theta - C_e) - \phi_e \theta$$

$$\Theta = \frac{(\theta - \mathcal{H})}{St}(-d_c\theta - C_e) - \left(1 - \frac{\theta - \mathcal{H}}{St}\right)\theta$$

$$St\,\Theta = (\theta - \mathcal{H})(-d_c\theta - C_e) - (St - \theta + \mathcal{H})\theta .$$

$$St\,\Theta = -d_c\theta^2 + d_c\theta\mathcal{H} - \theta C_e + C_e\mathcal{H} - (St + \mathcal{H})\theta + \theta^2$$

$$St\,\Theta = \theta^2(1-d_c) + \theta(d_c\mathcal{H} - C_e - St - \mathcal{H}) + C_e\mathcal{H}.$$

$A\theta^2 - B\theta + C = 0 \qquad B \qquad C$

$$\theta^2(1-d_c) - \theta\left((1-d_c)\mathcal{H} + C_e + St\right) + C_e\mathcal{H} - St\,\Theta = 0$$

$$\theta = \frac{B \pm \sqrt{B^2 - 4AC}}{2A}$$

$$B^2 - 4AC = \left[(1-d_c)\mathcal{H} + C_e + St\right]^2 - 4(1-d_c)(C_e\mathcal{H} - St\,\Theta)$$

This is always true.

to get a -ve temperature must take -ve root

so $\theta = \dfrac{B - \sqrt{B^2-4AC}}{2A}$. $\Theta_e = -\theta$

$\Theta_s = -d_c\theta - C_e$

$\phi_l = 1 - \dfrac{\theta - \mathcal{H}}{St}$ $\phi_g = 0$, $\phi_s = 1 - \phi_l$, $\omega = \dfrac{\Gamma}{\chi\phi_l}$.

$\mathcal{H}_L$ Boundary: $\phi_g = 0$ $\phi_s = 0$ $\phi_l = 1$

$\ominus$ $\theta = -\Theta_e$ $\Theta_s = -d_c\theta - C_e$.

$\mathcal{H}_L = \theta$ so $\mathcal{H}_L^-(\Theta) = -\Theta$.

$\Theta = -\theta$.

Eutectic Region $\ominus$ $\theta = \theta_s(\Theta_s)$, $\Theta_l = 1$, $\phi_g = 0$

$\omega = \Gamma / \chi\phi_l$ $\phi_s = 1 - \phi_l$.

need Θ_s & ϕ_l

$\mathcal{H} = \theta - (1-\phi_l)St$.

$\Theta = (1-\phi_l)\Theta_s + \phi_l$

we actually always have that $\Theta_s > C_c - C_e$
so $\theta = -1$
otherwise we intersect the solidus.

so $\mathcal{H} = -1 - (1-\phi_l)St$

$\Theta = (1-\phi_l)\Theta_s + \phi_l$

so $\dfrac{\mathcal{H}+1}{St} = \phi_l - 1$ so $\phi_l = \dfrac{\mathcal{H}+1}{St} + 1$

and $\phi_s = -\dfrac{(\mathcal{H}+1)}{St}$.

$\Theta_s = \dfrac{\Theta - \phi_l}{1-\phi_l}$, $\theta = -1$.

H_E ⊖ Bandy: $\theta = -1$, $\Theta_l = 1$, $\phi_g = 0$, $\Theta_S = d_c - e_e$.

$\omega = \Gamma / \chi\phi_l$ $\phi_S = 1 - \phi_l$.

$H_E = -1 - (1-\phi_l)St$

$\Theta = \phi_l + (1-\phi_l)(d_c - e_e)$.

$\phi_l^E (1 - d_c + e_e) + (d_c - e_e) = \Theta$

$$\phi_l^E = \frac{\Theta + e_e - d_c}{1 - d_c + e_e}$$

$H_E^-(\Theta) = -1 - St(1 - \phi_l^E(\Theta))$.

intersect solidus at $\Theta = d_c - e_e$.

intersect liquidus at $\Theta = 1$.

H_S ⊖ Bandy: $\theta = \theta_S(\Theta_S)$, $\phi_l = 0$, $\phi_g = 0$

$\Theta_l = 1$, $\omega = \Gamma / \chi\phi_l$, $\phi_S = 1$.

$H_S = \theta_S - St$

$\Theta = \Theta_S$ so $H_S^- = \max(-1 - St, \frac{-1}{d_c}(\Theta + e_e) - St)$.

Solid Region $\phi_s = 1$, $\phi_g = 0$, $\phi_l = 0$, $\Theta_e = 1$

$\omega = 1$ (continuity).

$H = \Theta - St$

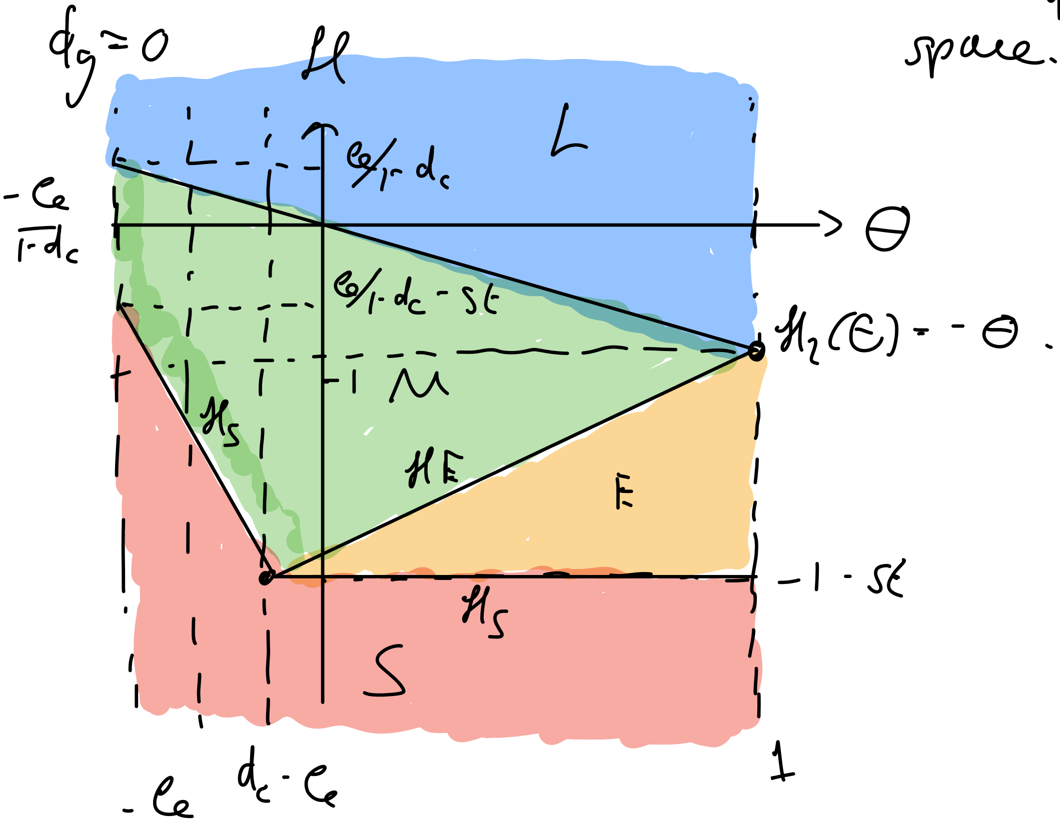
$\Theta = \Theta_s$

$\Theta = H + St$, $\Theta_s = \Theta$.

$\Gamma < \Gamma_{sat} = \chi \phi_e(H, \Theta)$

phase diagram in enthalpy space.

$\phi_g = 0$



Now do same calculations with

$\Gamma > \Gamma_{sat}$

so $\omega = 1$ & $\phi_g > 0$

These should match up as $\phi_g \to 0$

Liquid Region: $\phi_S = 0$, $\Theta_S = d_c\Theta_e - \mathcal{C}_e$, $\omega = 1$

$\phi_l = 1 - \phi_g$ $\oplus$

$$\mathcal{H} = \Theta(1-\phi_g)$$

$$\Theta = (1-\phi_g)\Theta_e - \frac{\phi_g \mathcal{C}_e}{1-d_c}$$

$\Gamma = \chi(1-\phi_g) + \phi_g$ $\quad \phi_g(1-\chi) = \Gamma - \chi$

so $\phi_g = \dfrac{\Gamma - \chi}{1-\chi}$ (Note $\chi \leq \Gamma \leq 1$)

we kn $\phi_S, \Theta_S, \phi_g, \omega$

$\Rightarrow \phi_l = 1 - \phi_g$ known

need Θ_l & Θ

$$\Theta = \mathcal{H}/_{1-\phi_g} \qquad \Theta_l = \frac{\Theta + \frac{\phi_g \mathcal{C}_e}{1-d_c}}{1-\phi_g}$$

Mushy Regin Θ : $\omega=1$, $\theta = -\Theta_e$, $\mathcal{G}_s = d_c \mathcal{G}_e - \mathcal{C}_e$.

$\Gamma = \chi\phi_e + \phi_g$ so $\phi_g = \Gamma - \chi\phi_l$. $\phi_s = 1-\phi_e - \phi_g$

need ϕ_l & θ

$$\mathcal{H} = \theta(1-\phi_g) - (1-\phi_l - \phi_g)St.$$

$$\Theta = -\phi_e\theta + (1-\phi_e - \phi_g)(-d_c\theta - \mathcal{C}_e) - \frac{\phi_g \mathcal{C}_e}{1-d_c}.$$

$$\Theta = -\phi_l\theta + \phi_s(-d_c\theta - \mathcal{C}_e) - \frac{\phi_g \mathcal{C}_e}{1-d_c}$$

$$\mathcal{H} = \theta(1-\phi_g) - \phi_s St$$

so $$\boxed{\frac{\mathcal{H} + \phi_s St}{(1-\phi_g)} = \theta}$$

Find ϕ_l in terms of θ assumming $\underline{d_c = 0}$

$$\mathcal{H} = \theta(1-\Gamma + \chi\phi_e) - (1-\phi_l - \Gamma + \chi\phi_l)St$$

$$\Theta = -\phi_l\theta - (1-\phi_l - \Gamma + \chi\phi_l)\mathcal{C}_e - \mathcal{C}_e(\Gamma - \chi\phi_l)$$

$$\Theta = -\phi_l\theta - \mathcal{C}_e(1-\phi_l)$$

so $\Theta = \phi_l(-\theta + \mathcal{C}_e) - \mathcal{C}_e$ so $$\boxed{\phi_l = \frac{\Theta + \mathcal{C}_e}{\mathcal{C}_e - \theta}}$$

Mathematica finds 2 solutions for θ.

$$\theta_1 = -\frac{1}{2A}\left(B - \sqrt{4AC + E^2}\right)$$

solution of

$$\theta_2 = -\frac{1}{2A}\left(B + \sqrt{4AC + E^2}\right)$$

$$A\theta^2 - B\theta - C = 0$$

First show $B = E$

$$B = \mathcal{C}_e + \mathcal{H} + St - \mathcal{C}_e\Gamma - St\Gamma + \mathcal{C}_e\chi + \mathcal{L}_i\chi - \mathcal{C}_e d_c$$
$$- 2\mathcal{H}d_c - St\,d_c + \mathcal{C}_e\Gamma d_c + St\Gamma d_c + \mathcal{H}\chi d_c$$
$$- \mathcal{L}_i\chi d_c + \mathcal{H}d_c^2 - \mathcal{H}\chi d_c^2$$

Factorise by d_c

$$B = \mathcal{C}_e + \mathcal{H} + St - \mathcal{C}_e\Gamma - St\Gamma + \mathcal{C}_e\chi + \mathcal{L}_i\chi$$
$$+ d_c\left(-\mathcal{C}_e - 2\mathcal{H} - St + \mathcal{C}_e\Gamma + St\Gamma + \mathcal{H}\chi - \mathcal{L}_i\chi\right)$$
$$+ d_c^2\left(\mathcal{H} - \mathcal{H}\chi\right)$$

$B = E$ confirmed group by the new

$$B = G_e(1 - \Gamma + \chi - d_c + \Gamma d_c)$$
$$+ H(1 - 2d_c + \chi d_c + d_c^2 - \chi d_c^2)$$
$$+ G_i(\chi)(1 - d_c)$$
$$+ St(1 - \Gamma - d_c + \Gamma d_c)$$

$$B = G_e(1 - d_c - \Gamma(1 - d_c) + \chi)$$
$$+ H((1 - d_c)^2 + \chi d_c(1 - d_c))$$
$$+ G_i \chi(1 - d_c)$$
$$+ St(1 - d_c - \Gamma(1 - d_c))$$

$$B = G_e((1 - d_c)(1 - \Gamma) + \chi)$$
$$+ H(1 - d_c)(1 - d_c + \chi d_c)$$
$$+ G_i \chi(1 - d_c)$$
$$+ St(1 - d_c)(1 - \Gamma)$$

$$B = (1-d_c)\left[(C_e + St)(1-\Gamma) + \mathcal{H}(1-d_c+d_c\chi) + \Gamma_i\chi\right] + C_e\chi$$

$$\theta_1 = -\frac{1}{2A}\left(B - \sqrt{4AC+B^2}\right)$$

$$\theta_2 = -\frac{1}{2A}\left(B + \sqrt{4AC+B^2}\right)$$

$$A = (\Gamma-1)(d_c-1)^2$$

$$C = St\,\Gamma_i(\chi-1) + C_e(\mathcal{H} - St\,\Gamma + St\,\chi)$$
$$+ (C_e\mathcal{H} - St\,\Gamma_i)d_c(\chi-1)$$

$$= St\,\Gamma_i\chi - St\,\Gamma_i + C_e\mathcal{H} - St\,C_e\Gamma + C_e\,St\,\chi$$
$$+ C_e\mathcal{H}d_c(\chi-1) - St\,\Gamma_i d_c(\chi-1)$$

$$C = St\,\Gamma_i\left((\chi-1) - d_c(\chi-1)\right)$$
$$+ C_e\mathcal{H}\left(1 + d_c(\chi-1)\right)$$
$$+ St\,C_e(\chi-\Gamma)$$

$$C = St\Gamma_1(1-d_c)(\chi-1)$$
$$+ C_e H((1-d_c)+d_c\chi)$$
$$+ St\, C_e(\chi-\Gamma)$$

$$C = (1-d_c)\left[(\chi-1)St\Gamma_1 + C_e H\right] + d_c C_e H\chi$$
$$+ St\, C_e(\chi-\Gamma).$$

$$C = (1-d_c)\left[C_e H - (1-\chi)St\Gamma_1\right] + C_e\left[d_c H\chi - St(\Gamma-\chi)\right]$$

in the limit $\Gamma = \chi = 0$

$$C = (1-d_c)\left[C_e H - St\Gamma_1\right]$$
$$A = -(1-d_c)^2$$
$$B = (1-d_c)\left[C_e + St + H(1-d_c)\right]$$

Agrees with previous work

Nale

Note $\theta_1 = -\frac{1}{2A}\left(B - \sqrt{B^2+4AC}\right)$

$\theta_2 = -\frac{1}{2A}\left(B + \sqrt{B^2+4AC}\right)$

in limit $\Gamma = \chi = 0$

$d_c = 0$

$C = e_e H - \delta t \Sigma_1^\dagger$

$A = -1 < 0$

$B = e_e + \delta t + H$

in Mu2 $H < -\Sigma_1^\dagger$

$-e_e < \Sigma_1^\dagger < 1$. $\quad e_e > -\Sigma_1^\dagger > -1$

$-1 < -\Sigma_1^\dagger < e_e$.

so most -ve H is $H = -1$

lowest value of B is $e_e + \delta t - 1 > 0$.

so $B > 0$.

to get a negative temp Take θ_1!

$\theta_1 = \frac{1}{2}\left(B - \sqrt{\cdots}\right) \quad \theta_2 = \frac{1}{2}\left(B + \sqrt{\cdots}\right)$

renamed

$\Theta = \Sigma_1^\dagger$

TLDR :

$$\theta = -\frac{1}{2A}\left(B - \sqrt{B^2+4AC}\right)$$

$$A = (\Gamma-1)(1-d_c)^2$$

$$B = (1-d_c)\left[(\mathcal{C}_e+St)(1-\Gamma) + \mathcal{H}(1-d_c+d_c\chi) + \mathcal{C}_1\chi\right] + \mathcal{C}_e\chi$$

$$C = (1-d_c)\left[\mathcal{C}_e\mathcal{H} - (1-\chi)St\,\mathcal{C}_1\right] + \mathcal{C}_e\left[d_c\mathcal{H}\chi - St(\Gamma-\chi)\right]$$

in Supersaturated + Mushy Region.

Liquidus Bdry: $\omega = 1$, $\phi_s = 0$, $\Theta_s = d_c \Theta_e - c_e$.

$$\theta = -\Theta_l.$$

$$\phi_l = 1 - \phi_g$$

$$\mathcal{H}_L^+ = \theta(1-\phi_g)$$

$$\Theta = (1-\phi_g)(-\theta) - \frac{\phi_g c_e}{1-d_c}.$$

$$\Gamma = \phi_g + \chi(1-\phi_g) \qquad \phi_g = \frac{\Gamma - \chi}{1-\chi}.$$

ϕ_g is known

$$\frac{\Theta + \frac{\phi_g c_e}{1-d_c}}{1-\phi_g} = -\theta.$$

so $\mathcal{H}_L^+(\Theta) = -\left(\Theta + \frac{\phi_g c_e}{1-d_c}\right).$

Eutectic Region: $\omega = 1 \quad \theta = -1, \quad \theta_e = 1,$

$$\mathcal{H} = -1(1-\phi_g) - (1-\phi_l-\phi_g)St. \qquad \phi_s = 1-\phi_l-\phi_g$$

$$\Theta = \phi_l + (1-\phi_l-\phi_g)\Theta_S - \frac{\phi_g C_e}{1-d_c}$$

$$\Gamma = \chi\phi_l + \phi_g. \qquad \phi_g = \Gamma - \chi\phi_l$$

solve for ϕ_l, ϕ_g, Θ_S

$$\Theta_S = \frac{\Theta + \frac{\phi_g C_e}{1-d_c} - \phi_l}{1-\phi_l-\phi_g}$$

$$\mathcal{H} = \phi_g - 1 - (1-\phi_l-\phi_g)St$$

$$\mathcal{H} = \Gamma - \chi\phi_l - 1 - (1-\phi_l-\Gamma+\chi\phi_l)St.$$

$$\mathcal{H} = \phi_l(-\chi + St - \chi St) + \Gamma - 1 - St + \Gamma St.$$

$$\mathcal{H} = \phi_l(St(1-\chi) - \chi) - (1-\Gamma)(1+St)$$

$$\phi_l = \frac{(1-\Gamma)(1+St) + \mathcal{H}}{St(1-\chi) - \chi}$$

$$\phi_g = \Gamma - \chi\phi_l .$$

Eutectic Boundary$^+$: $\omega = 1,\ \theta = -1,\ \theta_l = 1$

$\theta_s = d_c - C_e$

$$\phi_s + \phi_l + \phi_g = 1$$

$$\mathcal{H}_E^+ = -1(1-\phi_g) - \phi_s St$$

$$\theta = \phi_l + \phi_s(d_c - C_e) - \frac{\phi_g C_e}{1-d_c}$$

$$\Gamma = \phi_e \chi + \phi_g$$

$d_c = 0$

$$\phi_g = \Gamma - \phi_e \chi$$

$$\phi_s = 1 - \phi_g - \phi_e = 1 - \Gamma + \phi_e\chi - \phi_e$$

$$\theta = \phi_e - C_e(1 - \Gamma + \phi_e\chi - \phi_e) - C_e(\Gamma - \phi_e\chi)$$

$$\theta = \phi_l(1 - C_e\chi + C_e + C_e\chi)$$
$$+ C_e\Gamma - C_e - C_e\Gamma$$

$$\theta = \phi_l(1 + C_e) - C_e$$

$\phi_l = \dfrac{\theta + C_e}{1 + C_e}$ same as before

but now $\phi_g = \Gamma - \dfrac{\chi(\theta + C_e)}{1 + C_e}$

$$H_E^+(\theta, \Gamma) = -1(1 - \phi_g) - \phi_s St$$

at $\theta = -C_e$ $\phi_l = 0$ $\phi_g = \Gamma$, $\phi_s = 1 - \Gamma$ ✓

$$H_E^+ = -1(1 - \Gamma + \chi\phi_l^E) - (1 - \phi_l^E - \Gamma + \chi\phi_l^E)St$$
$$H_E^+ = -1(1 - \Gamma + \chi\phi_l^E) - St(1 - \Gamma + \phi_l^E(\chi - 1)).$$

Solidus Boundary: $\phi_l = 0$, $\omega = 1$, $\theta = \theta_S$, θ_l N/A

$\oplus$

$$H_S^+ = (1 - \phi_g)\theta_S - (1 - \phi_g)St = (1 - \phi_g)(\theta_S - St)$$

$$\theta = (1 - \phi_g)\theta_S - \frac{\phi_g C_e}{1 - \phi_c} \qquad \Gamma = \phi_g$$

$$\Theta_s = \frac{\Theta + \frac{r\ell_e}{1-d_c}}{1-r}$$

$$\theta_s(\Theta_s) = \max\left(-1,\ -\tfrac{1}{d_c}(\Theta_s + \ell_e)\right)$$

$$\theta_s(\Theta_s) = \begin{cases} -1, & \Theta_s > d_c - \ell_e \\ -\frac{1}{d_c}(\Theta_s + \ell_e), & \Theta_s \leq d_c - \ell_e \end{cases}$$

$$\theta_s = \max\left(-1,\ \frac{-1}{d_c}\left(\frac{\Theta + \frac{r\ell_e}{1-d_c}}{1-r} + \ell_e\right)\right).$$

so $\mathcal{H}_s^+(\Theta) = (1-r)\max\left(-1-St,\ \frac{-1}{d_c}\left(\frac{\Theta + \frac{r\ell_e}{1-d_c}}{1-r} + \ell_e\right) - St\right).$

Solid Region ⊕: $\phi_l = 0$, θ_l N/A, $\omega = 1$

$$\mathcal{H} = \theta(1-\phi_g) - (1-\phi_g)St = (1-\phi_g)(\theta - St)$$

$$\Theta = \phi_s\theta_s - \frac{\phi_g\ell_e}{1-d_c} = (1-r)\theta_s - \frac{r\ell_e}{1-d_c}$$

$$r = \phi_g$$

$$\sigma_s = \frac{\sigma + \frac{ru}{1-d_c}}{1-n}$$

$$\theta = \frac{u}{1-n} + St$$

$$\phi_g = n$$

$$\phi_s = 1-n$$

Calculating Phase Boundaries.

Need total phase boundaries

$$\mathcal{H}_{L,E,S}(\Theta, \Gamma) \quad \& \quad \Gamma_{sat}(\mathcal{H}, \Theta).$$

Note that for $\Gamma \leq \Gamma_{sat}$ phase boundaries are independent of Γ

$$\therefore \quad \Gamma_{sat}(\mathcal{H}, \Theta) = \chi \phi_l(\mathcal{H}, \Theta).$$

where $\phi_l = \phi_l$ subsaturated

$$\Gamma_{sat}(\mathcal{H}, \Theta) = \begin{cases} \chi & \mathcal{H} \geq \mathcal{H}_L^-(\Theta) \\ \chi\left(1 - \left(\frac{\theta - \mathcal{H}}{St}\right)\right), & \mathcal{H}_E^-(\Theta) \leq \mathcal{H} < \mathcal{H}_L^-(\Theta) \\ \chi\left(1 + \left(\frac{\mathcal{H}+1}{St}\right)\right), & \mathcal{H}_S^- \leq \mathcal{H} \leq \mathcal{H}_E^-(\Theta) \\ 0, & \mathcal{H} \leq \mathcal{H}_S^-(\Theta) \end{cases}$$

where

$$\theta = \frac{B - \sqrt{B^2 - 4AC}}{2A}$$

$A = 1 - d_c$

$B = (1 - d_c)\mathcal{H} + \mathcal{C}_e + St$

$C = \mathcal{C}_e\mathcal{H} - St\,\Theta$

$$\mathcal{H}_L^-(\Theta) = -\Theta$$

$$\phi_l^E = \frac{\Theta + \mathcal{C}_e - d_c}{1 - d_c + \mathcal{C}_e}$$

$$\mathcal{H}_E^-(\Theta) = -1 - St(1 - \phi_l^E(\Theta)).$$

$$\mathcal{H}_S^- = \max\left(-1 - St, \frac{-1}{d_c}(\Theta + \mathcal{C}_e) - St\right).$$

To calculate
phase boundaries we need intersection with Γ_{sat}

occurs at $\Gamma_L^{sat} = \Gamma_{sat}(\mathcal{H}_L^-(\Theta), \Theta)$

$$\Gamma_E^{sat} = \Gamma_{sat}(\mathcal{H}_E^-(\Theta), \Theta)$$

$$\Gamma_S^{sat} = \Gamma_{sat}(\mathcal{H}_S^-(\Theta), \Theta)$$

then $\mathcal{H}_L(\Theta, \Gamma) = \begin{cases} \mathcal{H}_L^-(\Theta) & , \Gamma \le \Gamma_L^{sat}(\Theta) \\ \mathcal{H}_L^+(\Theta, \Gamma) & , \Gamma > \Gamma_L^{sat}(\Theta) \end{cases}$

same for E & S.

when $\mathcal{H} = \mathcal{H}_L^-(\Theta)$ $\Gamma_L^{sat} = \chi$

when $\mathcal{H} = \mathcal{H}_S^-(\Theta)$ $\Gamma_S^{sat} = 0$

$\mathcal{H} = \mathcal{H}_E^-(\Theta)$ $\Gamma_E^{sat} = \chi\left(\frac{\Theta + c_e - d_c}{1 - d_c + c_e}\right)$

$$\mathcal{H}_E^- = -1 - St(1 - \phi_1^E(\Theta))$$

$$\Gamma_E^{sat} = \chi\left(1 - (1 - \phi_1^E(\Theta))\right)$$

$$= \chi \phi_1^E(\Theta) = \chi\left(\frac{\Theta + c_e - d_c}{1 - d_c + c_e}\right)$$

$$H_L(\theta,\Gamma) = \begin{cases} -\theta, & \Gamma \le \chi \\ -\left(\theta + \frac{C_e}{1-d_c}\left[\frac{\Gamma-\chi}{1-\chi}\right]\right), & \Gamma > \chi \end{cases}$$

$$H_E(\theta,\Gamma) = \begin{cases} -1 - St\left(1-\phi_l^E(\theta)\right), & \Gamma \le \chi\phi_l^E(\theta) \\ -1(1-\phi_g) - \phi_s St, & \Gamma > \chi\phi_l^E(\theta) \end{cases}$$

$\phi_l^E = \dfrac{\theta + C_e}{1+C_e}$ same as before $(d_c = 0)$

$(\Gamma - \chi\phi_l^E)$

$\phi_s = 1 - \phi_l^E - \phi_g \qquad \phi_g = \Gamma - \dfrac{\chi(\theta+C_e)}{1+C_e}$

$$H_S(\theta,\Gamma) = \begin{cases} \max\left(-1-St, -\frac{1}{d_c}(\theta+C_e) - St\right), & \Gamma = 0 \\ (1-\Gamma)\max\left(-1-St, -\frac{1}{d_c}\left(\frac{\theta + \frac{\Gamma C_e}{1-d_c}}{1-\Gamma} + C_e\right) - St\right), & \Gamma > 0 \end{cases}$$

Bounds: H can be anything.

$0 \le \Gamma \le 1$.

$-\dfrac{C_e}{(1-d_c)} \le \theta \le \theta_{max} = 1 - \phi_g\left(1 + \dfrac{C_e}{1-d_c}\right)$

bulk fresh

the reduced eutectic point for a given ϕ_g $\theta_{max}(\phi_g)$

s.t. $\theta_{max}(0) = 1$.

To plot $\theta_{max}(\Gamma)$

we can use defined in liquid $f_g = \frac{\Gamma - \chi}{1-\chi}$.

$\Gamma \geq \chi$;

$\Gamma < \chi$ $f_g = 0$

$$\theta_{max} = \begin{cases} 1, & \Gamma \leq \chi \\ 1 - \left(\frac{\Gamma - \chi}{1-\chi}\right)\left(1 + \frac{c_e}{1-d_c}\right), & \Gamma > \chi. \end{cases}$$

References

[1] R. F. Katz and M. G. Worster, “Simulation of directional solidification, thermochemical convection, and chimney formation in a Hele-Shaw cell,” *Journal of Computational Physics*, vol. 227, pp. 9823–9840, Dec. 2008.