Formulating the Moving Boundary Problem

(or Conservation of Mass: It isn't just a good idea, it's the law)

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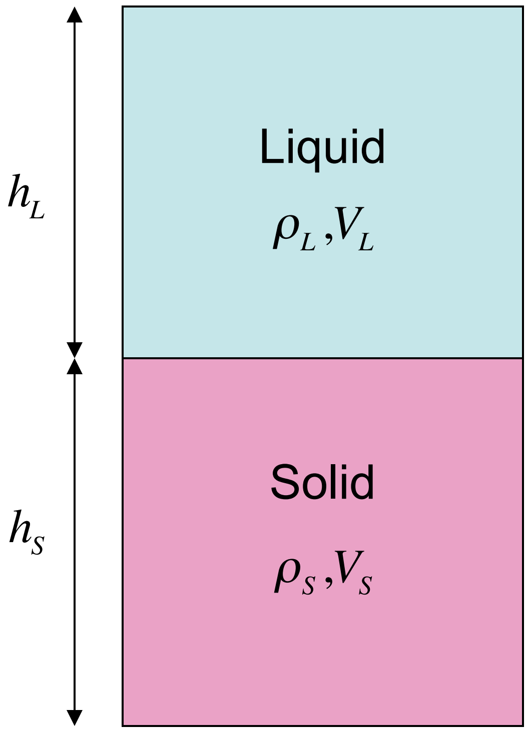
Solidification from the melt



Global mass conservation

$$\rho_L V_L + \rho_S V_S = M$$

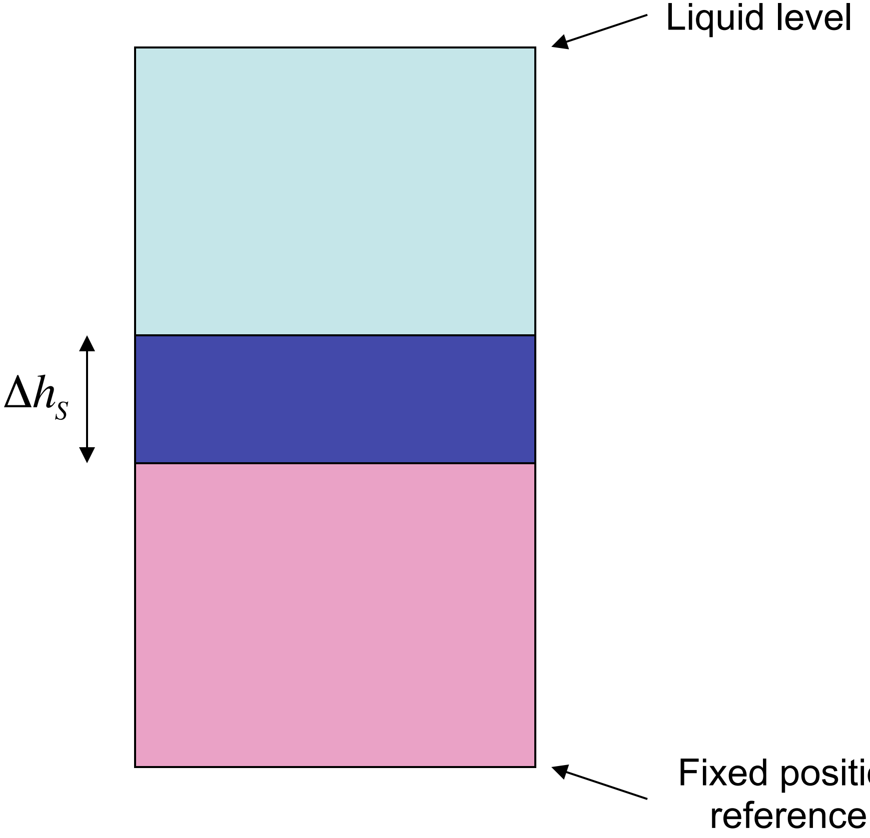
Time rate of change

$$\rho_L \frac{dV_L}{dt} + \rho_S \frac{dV_S}{dt} = \frac{dM}{dt} = 0$$

Simplify to one-dimensional case

$$\rho_L \frac{dh_L}{dt} + \rho_S \frac{dh_S}{dt} = 0$$

Case 1: Equal densities



Rearrange

$$\frac{dh_L}{dt} = -\frac{\rho_S}{\rho_L}\frac{dh_S}{dt}$$

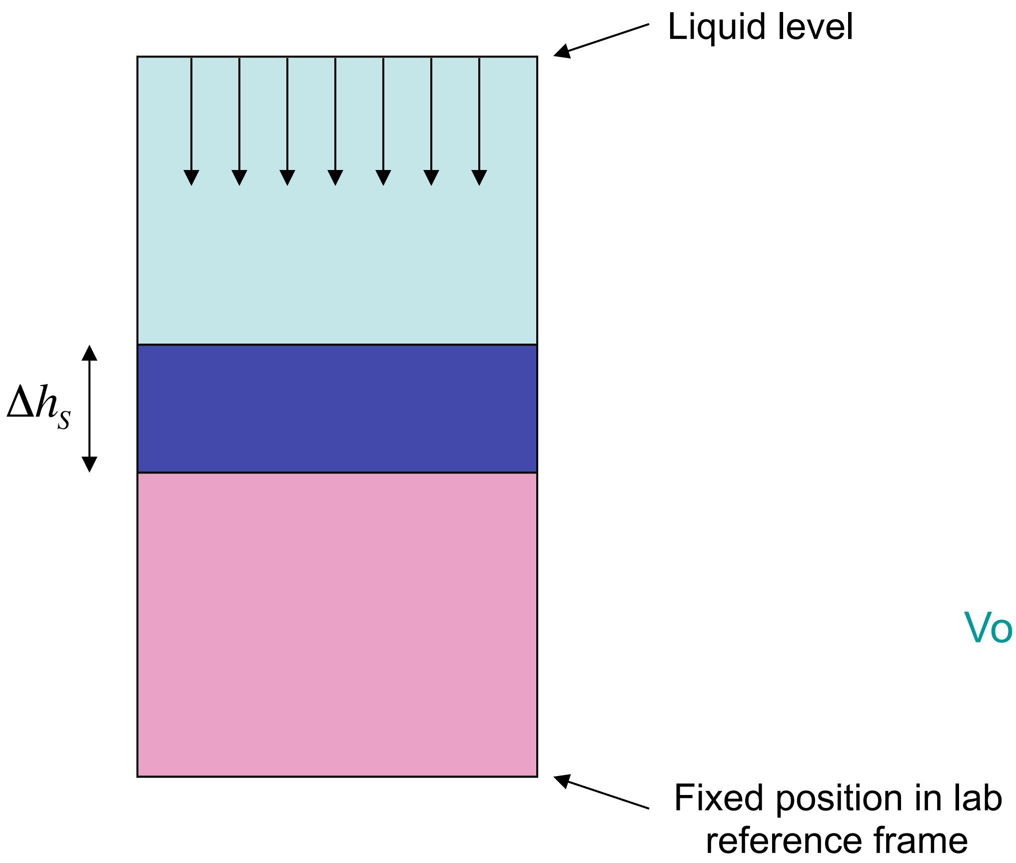
or

$$\frac{dh_L}{dt} = -\frac{dh_S}{dt}$$

Volume of liquid lost equals volume of solid gained

Equal densities: Liquid level remains constant

Case 2: Unequal densities



Rearrange

$$\frac{dh_L}{dt} = -\frac{\rho_S}{\rho_L}\frac{dh_S}{dt}$$

Consider

$$\rho_S > \rho_L$$

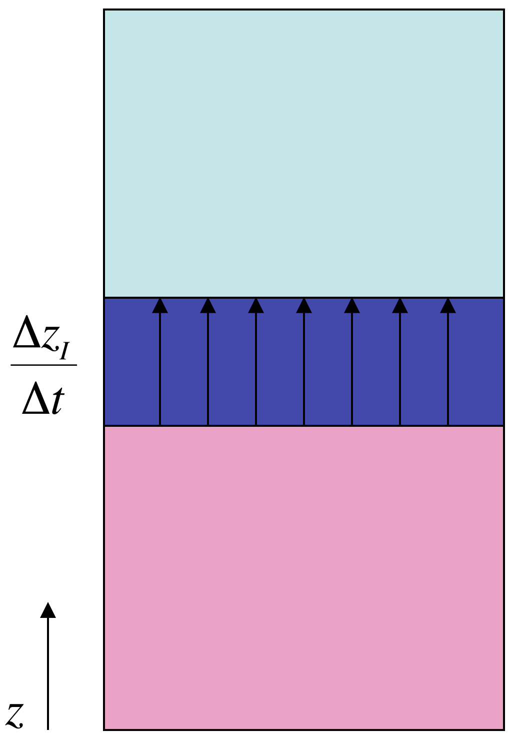
$$\frac{dh_L}{dt} > -\frac{dh_S}{dt}$$

Volume of liquid lost exceeds volume of solid gained

Unequal densities: Liquid level falls (rises) during growth

Flow boundary conditions: Equal densities

Introduce a coordinate z relative to bottom of solid



Interface moves at velocity = $\frac{dz_I}{dt}$

What is correct velocity boundary condition at interface?

Rigid boundary in motion: $U = \frac{dz}{dt}$

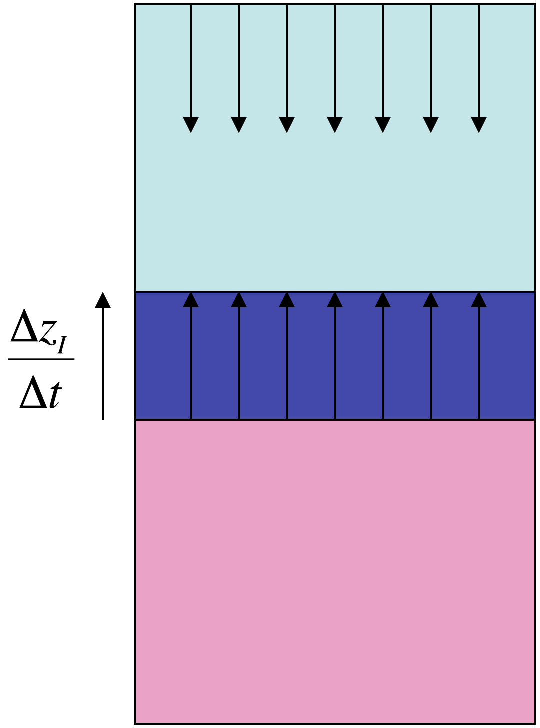
Volume of liquid lost equals volume of solid gained

- *Interface is not a rigid boundary*
- *Interface overtakes liquid*
- *Liquid is solidified in place*
- *No-slip is correct boundary condition*

$$U = 0$$

Interface motion does not induce any motion of liquid

Flow boundary conditions: Unequal densities



Derivation 1

Mass of solid created $\rho_S \Delta z_I$

Mass of liquid overtaken $\rho_L \Delta z_I$

Mass shortage $\rho_S \Delta z_I - \rho_L \Delta z_I$

Liquid must flow downward to make up shortfall

$$\rho_L U \Delta t = \rho_L \Delta z_I - \rho_S \Delta z_I$$

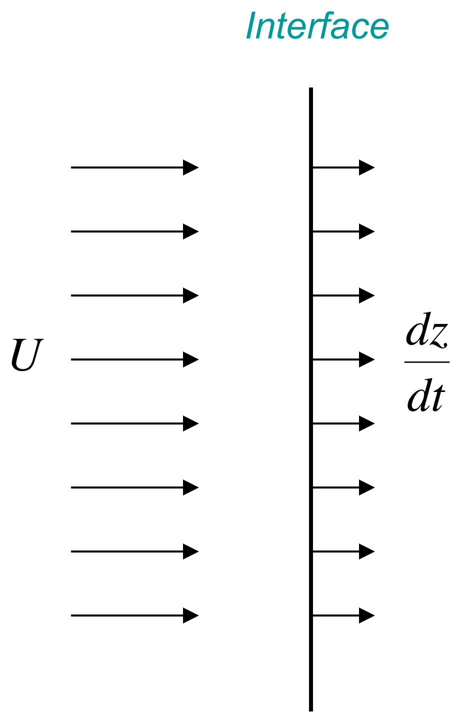
Rearrange, $\Delta t \to 0$

$$U_I = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

By continuity, downward flow is uniform everywhere $(\rho_S > \rho_L)$

Flow boundary conditions: Unequal densities

Derivation 2



Mass crossing a moving interface

$$\rho\left(U - \frac{dz}{dt}\right)$$

Mass balance across interface

$$\rho_S\left(U_{S,I} - \frac{dz_I}{dt}\right) = \rho_L\left(U_{L,I} - \frac{dz_I}{dt}\right)$$

Rearrange, set $U_{S,I} = 0$

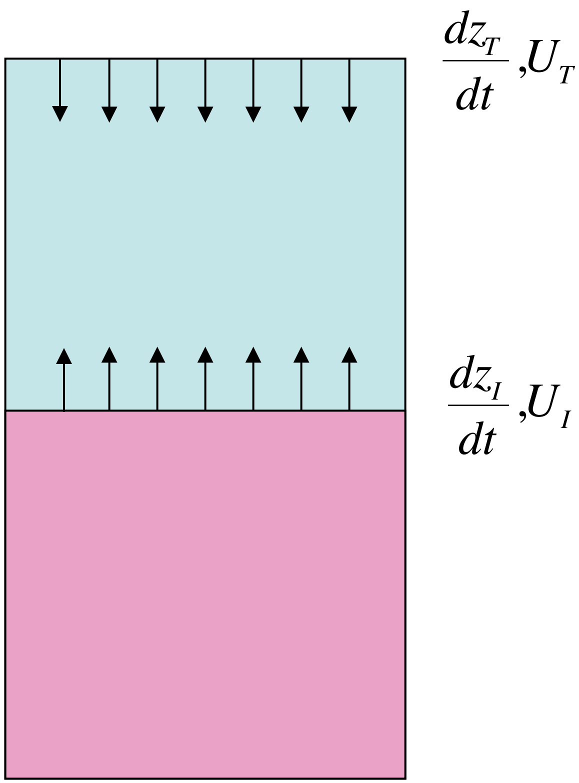
$$U_{L,I} = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

For equal density case $\rho_S = \rho_L \rightarrow U = 0$

By continuity, downward flow is uniform everywhere $(\rho_S > \rho_L)$

Rate of translation of interface and top boundary

Required information



Interface location set at melting point isotherm

$$T = T_{mp} \text{ constrains } z_I$$

$$\frac{\partial T}{\partial t} \text{ constrains } \frac{dz_I}{dt}$$

Mass balance at interface

$$U_I = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

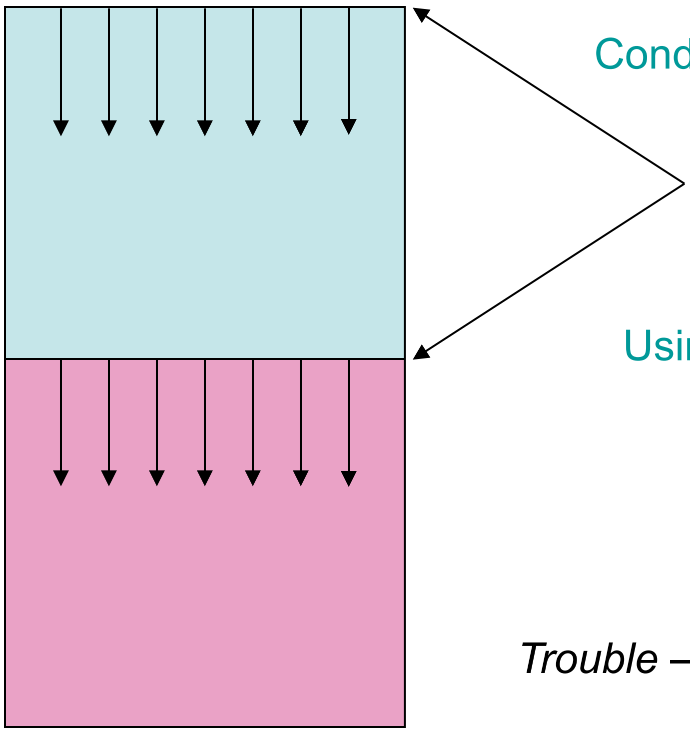
Top: rigid boundary in motion

$$U_T = \frac{dz_T}{dt}$$

We need one more relationship to complete the formulation

The global mass balance completes the picture

In this 1-D example, velocity is uniform everywhere



Condition at interface and top boundary

$$U_T = U_I = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

Using mass balance at top $\frac{dz_T}{dt} = U_T$

$$\frac{dz_T}{dt} = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

Trouble – BC at top is function of interface velocity

Conditions at top are non-local, destroys sparseness of discretization

Constraint-based approach to formulation

Use global mass balance directly

At interface

$$T = T_{mp}$$

$$U_I = \frac{dz_I}{dt}\left(1 - \frac{\rho_S}{\rho_L}\right)$$

At top boundary

$$U_T = \frac{dz_T}{dt}$$

Global mass conservation

$$\rho_L V_L + \rho_S V_S = M$$

More general, does not assume that flow is uniform everywhere

Generalization to 2- and 3-Dimensions

At interface	Melting point isotherm	$T = T_{mp}$
	Normal velocity	$\mathbf{n} \cdot \mathbf{u}_I = \mathbf{n} \cdot \frac{\partial \mathbf{x}_I}{\partial t}\left(1 - \frac{\rho_S}{\rho_L}\right)$
	Tangential velocity	$\mathbf{t} \cdot \mathbf{u_I} = 0$
At top boundary	Normal velocity	$\mathbf{n} \cdot \mathbf{u}_T = \mathbf{n} \cdot \frac{\partial \mathbf{x}_T}{\partial t}$
	Tangential velocity	$\mathbf{t} \cdot \mathbf{u}_T = 0$
Everywhere	Global mass conservation	$\rho_L V_L + \rho_S V_S = M$

Completely general in any number of dimensions, for non-uniform flow

Implementation of global constraint

Global mass conservation

$$\rho_L V_L + \rho_S V_S = M$$

Discretized form: element-by-element sum

$$\rho_L \sum_{N_L} \int_{\Omega_E} d\Omega_E + \rho_S \sum_{N_S} \int_{\Omega_E} d\Omega_E = M$$

Consequences

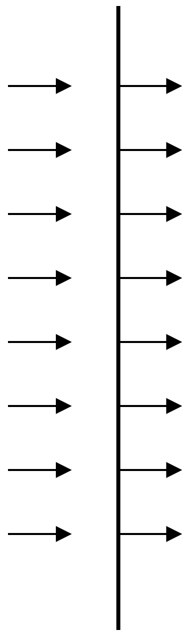
- Single residual, non-local, Jacobian has one dense row
- Easily solved using Sherman-Morrison or Woodbury technique
- Requires one additional back-substitution

Boundary conditions for mass transport – Segregation

Interface

Diffusion and convection

$$-D\mathbf{n}\cdot\nabla C + C\mathbf{n}\cdot\mathbf{u}$$



$$C\mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}$$

Mass crossing a moving interface

$$-D\mathbf{n}\cdot\nabla C + C\mathbf{n}\cdot\left(\mathbf{u}-\frac{\partial \mathbf{x}_I}{\partial t}\right)$$

Mass balance across interface

$$-D_S\mathbf{n}\cdot\nabla C_S + C_S\mathbf{n}\cdot\left(\mathbf{u}_S-\frac{\partial \mathbf{x}_I}{\partial t}\right)=$$

$$-D_L\mathbf{n}\cdot\nabla C_L + C_L\mathbf{n}\cdot\left(\mathbf{u}_L-\frac{\partial \mathbf{x}_I}{\partial t}\right)$$

Rearrange, use relations

$$C_S = k_p C_L,\;\; \mathbf{u}_S = 0,\;\; \mathbf{n}\cdot\mathbf{u}_L = \mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}\left(1-\frac{\rho_S}{\rho_L}\right)$$

Final result

$$-D_S\mathbf{n}\cdot\nabla C_S + D_L\mathbf{n}\cdot\nabla C_L = \mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}C_L\left(k_p-\frac{\rho_S}{\rho_L}\right)$$

Boundary conditions for mass transport – Top boundary

Mass balance at top boundary

$$-D_L \mathbf{n} \cdot \nabla C_L + C_L \mathbf{n} \cdot \left(\mathbf{u}_T - \frac{\partial \mathbf{x}_T}{\partial t} \right) = 0$$

Flow at top boundary

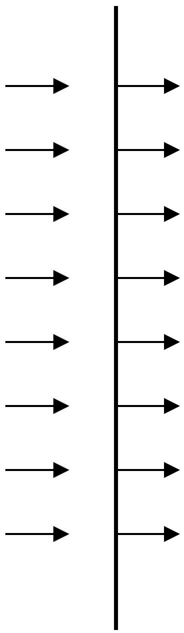
$$\mathbf{n} \cdot \mathbf{u}_T = \mathbf{n} \cdot \frac{\partial \mathbf{x}_T}{\partial t}$$

Final result

$$\mathbf{n} \cdot \nabla C_L = 0$$

Boundary conditions for heat transport

Interface



Conduction and convection

$$-k\mathbf{n}\cdot\nabla T + \rho H\mathbf{n}\cdot\mathbf{u}$$

$$\rho H\mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}$$

Heat balance across interface

$$-k_S\mathbf{n}\cdot\left(\nabla T\right)_S + \rho_S H_S\mathbf{n}\cdot\left(\mathbf{u}_S - \frac{\partial \mathbf{x}_I}{\partial t}\right) =$$

$$-k_L\mathbf{n}\cdot\left(\nabla T\right)_L + \rho_L H_L\mathbf{n}\cdot\left(\mathbf{u}_L - \frac{\partial \mathbf{x}_I}{\partial t}\right)$$

Rearrange, use relations

$$\mathbf{u}_S = 0,\ \ \mathbf{n}\cdot\mathbf{u}_L = \mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}\left(1-\frac{\rho_S}{\rho_L}\right)$$

Final result

$$-k_S\mathbf{n}\cdot\left(\nabla T\right)_S + k_L\mathbf{n}\cdot\left(\nabla T\right)_L =$$

$$\mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}\rho_S\left(H_S - H_L\right) = \mathbf{n}\cdot\frac{\partial \mathbf{x}_I}{\partial t}\rho_S\Delta H_f$$

Summary of boundary conditions/contraints

Interface	Melting point isotherm	$T = T_{mp}$
	Normal velocity	$\mathbf{n}\cdot\mathbf{u} = \mathbf{n}\cdot\dot{\mathbf{x}}\left(1-\rho_S/\rho_L\right)$
	Tangential velocity	$\mathbf{t}\cdot\mathbf{u} = 0$
	Segregation	$-D_S\mathbf{n}\cdot\nabla C_S + D_L\mathbf{n}\cdot\nabla C_L = \mathbf{n}\cdot\dot{\mathbf{x}}C_L\left(k_p-\rho_S/\rho_L\right)$
	Latent heat	$-k_S\mathbf{n}\cdot\left(\nabla T\right)_S + k_L\mathbf{n}\cdot\left(\nabla T\right)_L = -\mathbf{n}\cdot\dot{\mathbf{x}}\rho_S\Delta H_f$
Top boundary	Normal velocity	$\mathbf{n}\cdot\mathbf{u} = \mathbf{n}\cdot\dot{\mathbf{x}}$
	Tangential velocity	$\mathbf{t}\cdot\mathbf{u} = 0$
	Mass flux	$\mathbf{n}\cdot\nabla C_L = 0$
	Heat flux	$\mathbf{n}\cdot\nabla T = 0$
Everywhere	Global mass conservation	$\rho_L V_L + \rho_S V_S = M$