

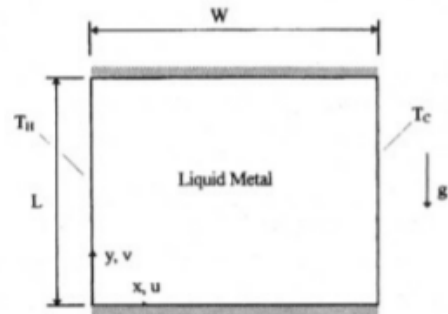
## GSoC SfePy

The final problem accounting convection-diffusion along with phase change has been defined below along with the governing equations and validation case studies.

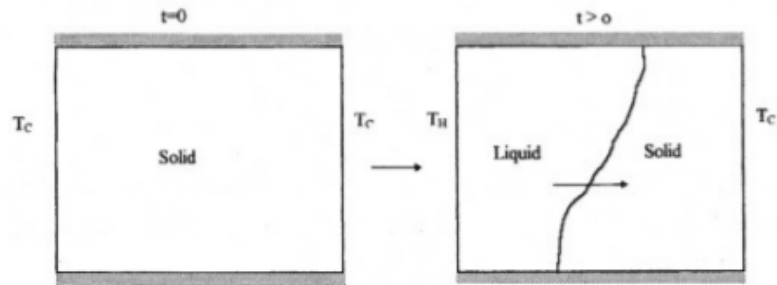
### Problem

Heat transfer in the processing of materials involving solid-liquid phase transformations (melting and solidification) is commonplace in such fields as metallurgy, crystal growth from melts and solutions, purification of materials, and solidification of metals. The associated density gradients in a gravitational field can induce natural convection flows. Convection in the liquid phase influences the process in two different ways, one of which is beneficial and the other of which can be detrimental. During melting convection increases the overall transport rate and, hence, the growth rate of the new phase, which is desirable. On the other hand, during solidification convection decreases the growth of the new phase and also seems to affect the morphology of the solid-liquid interface adversely. The nature of the solid is largely determined by what occurs in the vicinity of the solid-liquid interface. The heat release (absorption), density change, and other processes that take place in the vicinity of the transformation front result in nonuniformities along the front that cause its shape to change. The resulting density gradients in the liquid generate buoyancy-driven convection that can affect the transport of heat, constituent chemicals, and the growth rate.

The physical domain considered is shown in the figure. The vertical side walls of the enclosure are maintained at uniform temperatures, while the connecting horizontal walls are adiabatic. The governing equations are written for the entire domain assuming constant thermophysical properties, Boussinesq approximation, laminar, incompressible, and Newtonian two-dimensional flow. The solid-liquid interface motion due to volume change upon melting or solidification is neglected through the assumption  $\rho_s = \rho_l$ .



(a)



## Nomenclature

$\rho$	Density	$\text{kg/m}^3$
$\mu$	Viscosity	$\text{Pa}\cdot\text{s}$
$c_p$	Specific heat capacity	$\text{J/kg}\cdot\text{K}$
$k$	Thermal conductivity	$\text{W/m}\cdot\text{K}$
$\beta$	Thermal expansion coefficient	$1/\text{K}$
$L$	Latent heat of fusion	$\text{J/kg}$
$H$	Enthalpy	$\text{J/kg}$
$f$	Volume fraction	
$T$	Temperature	$^\circ\text{C}$
$t$	Time	$\text{s}$
$\vec{u}$	Velocity	$\text{m/s}$
$p$	Pressure	$\text{Pa}$
$S$	Source term	$\text{m/s}^2$

## Subscript

<i>l</i>	Liquid
<i>s</i>	Solid
<i>ref</i>	Reference
<i>eff</i>	Effective
<i>hot</i>	Hot
<i>cold</i>	Cold
<i>int</i>	Initial
<i>melt</i>	Melting

## Governing Equations

The continuum relations:

$$g_l + g_s = 1$$

$$f_l + f_s = 1$$

$$f_l = \frac{g_l \rho_l}{\rho}$$

$$f_s = \frac{g_s \rho_s}{\rho}$$

$$\rho = g_l \rho_l + g_s \rho_s$$

$$\vec{u} = f_l \vec{u}_l + f_s \vec{u}_s$$

$$k_{eff} = g_l k_l + g_s k_s$$

$$c_p = f_l c_{p_l} + f_s c_{p_s}$$

### 1. Continuity

$$\nabla \cdot (\vec{u}) = 0$$

### 2. Momentum

$$\rho \left[ \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right] = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{g} \beta (T - T_{ref}) + B \vec{u}$$

Now the key lies in modelling the source term. The coefficient  $B$  which should tend to 0 as the liquid volume fraction  $g_l$  approaches unity, and should become a large negative number to annihilate the motion in the fluid region at  $g_l = 0$ . Whereas these asymptotic conditions can be satisfied by several functions, we adopt the suggestion of Brent et al. :

$$B = \frac{-C(1 - g_l)^2}{(g_l^3 + b)}$$

where

$$C = 1.6 \times 10^6$$

$$b = 0.001$$

## 2. Energy

Writing a general equation for conservation of thermal energy for all the zones in the domain is facilitated by focusing on an element undergoing phase change. Below are the energy equation of solid and liquid phases under the thermal equilibrium condition  $T_l = T_s = T$ :

Solid

$$\frac{\partial(\rho_s g_s H_s)}{\partial t} + \nabla \cdot (\rho_s g_s \vec{u}_s H_s) = \nabla \cdot (g_s k_s \nabla T) + S_s$$

Liquid

$$\frac{\partial(\rho_l g_l H_l)}{\partial t} + \nabla \cdot (\rho_l g_l \vec{u}_l H_l) = \nabla \cdot (g_l k_l \nabla T) + S_l$$

where  $S_s$  and  $S_l$  are the interphase energy terms, having the same magnitude but being opposite in sign.

A single governing enthalpy equation results:

$$\frac{\partial(\rho H_m)}{\partial t} + \nabla \cdot \rho (f_s \vec{u}_s H_s + f_l \vec{u}_l H_l) = \nabla \cdot (k_{eff} \nabla T)$$

where

$$H_m = f_s H_s + f_l H_l = H_s + f_l (H_l - H_s)$$

The latent heat content of the element is due to the fraction of liquid converted to, or from, the corresponding quantity of solid. Hence we write

$$\Delta H = f_l (H_l - H_s) = f_l L$$

$$H_m = H_s + f_l L$$

$$H_s = c_p T$$

$$H_l = H_s + L$$

where  $L$  is the latent heat of fusion.

The zones where  $T > T_{melt}$ , the entire element is in the liquid state and  $f_l = 1$ .

The zones where  $T < T_{melt}$ , the entire element is in the solid state and  $f_l = 0$ .

It is the elements undergoing phase change at  $T = T_{melt}$ , where  $f_l$  varies between 0 and 1. Substituting  $H_m$  and  $H_l$  in equation we get

$$\frac{\partial(\rho H)}{\partial t} + \nabla \cdot (\rho \vec{u} H) = \nabla \cdot \left( \frac{k_{eff}}{c_p} \nabla H \right) S_e$$

where

$$\vec{u} = f_l \vec{u}_l$$

$$S_e = -\frac{\partial(\rho \Delta H)}{\partial t} = -\rho L \frac{\partial(f_l)}{\partial t}$$

### Initial Conditions

$f_l = 0$  everywhere  
 $T = T_{int}$  everywhere  
 $\vec{u} = 0$  everywhere.

### Boundary Conditions

$f_l = 1$  Left wall  
 $f_l = 0$  Right wall  
 $f_l[i][j] = f_l[i - 1][j]$  Top  
 $f_l[0][j] = f_l[1][j]$  Bottom  
 $T = T_{hot}$  Left wall  
 $T = T_{cold}$  Right wall  
 $\vec{u} = 0$  Walls

### Validation Cases

Melting Gallium : Gau and Viskanta  
Melting Gallium : Brent et al.  
Melting Calcium chloride : Zivkovic and Fujii

### References

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