Chapter 3

Phase change problems – Solidification & Melting

Introduction

- Materials processing, Metallurgy, purification of metals, growth of pure crystals from melts and solutions, solidification of casting and ingots, welding, electro-slag melting, zone melting, thermal energy storage using phase change materials, etc involve melting and solidification.
- These phase change processes are accompanied by either absorption or release of thermal energy.

Introduction cont..

- A moving boundary exists that separates the two phases of differing thermo-physical properties at which thermal energy is either absorbed or liberated.
- If we consider the solidification of casting or ingot, the superheat in the melt and the latent heat liberated at the solid-liquid interface are transferred across the solidified metal (interface and the mold) facing a certain thermal barrier at each of these stages.
- *Latent heat of fusion of a substance is the change in its enthalpy resulting from providing energy to a specific quantity of a substance to change its state from a solid to a liquid at a constant pressure.*

Introduction cont..

- The metal shrinks as it solidifies and an air gap is formed. Thus, additional thermal resistance is encountered. The heat transfer process occurring are complex.
- During the solidification of an alloy, the concentrations vary locally from the original mixture, as material may be physically incorporated or rejected at the solidification front. The material between the solidus and liquidus temperature is partly solid or partly liquid and resembles a porous medium and is referred as a “mushy zone”.

Classification of phase change types

- The nature of a solidification phase change can take many forms. An attempt to classify the possibilities is presented in Figure 1.
- This classification is based on the state of a small portion of the material in the phase change region, representing a single degree of freedom in the numerical discretization.
- Three classes of phase change are identified

Classification of phase change types

Case(a). Distinct:

The phase change region consists of distinct solid and liquid phases separated by a smooth continuous front; for example the freezing of water or rapid solidification of pure metals.

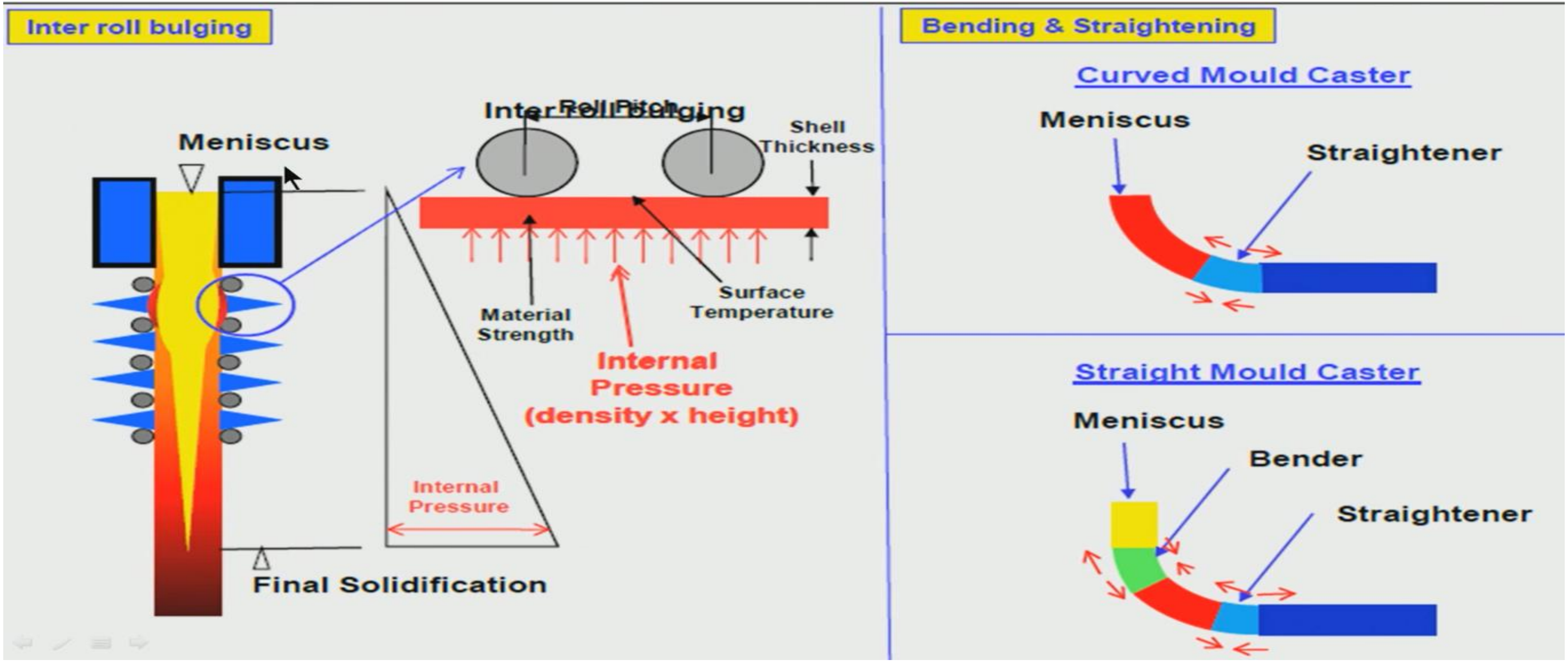
Case(b). Alloy:

The phase change region has a crystalline structure consisting of columnar and/or equi-axed grains and the solid/liquid interface is a complex shape not necessarily smooth or continuous; for example the solidification of most metal alloys.

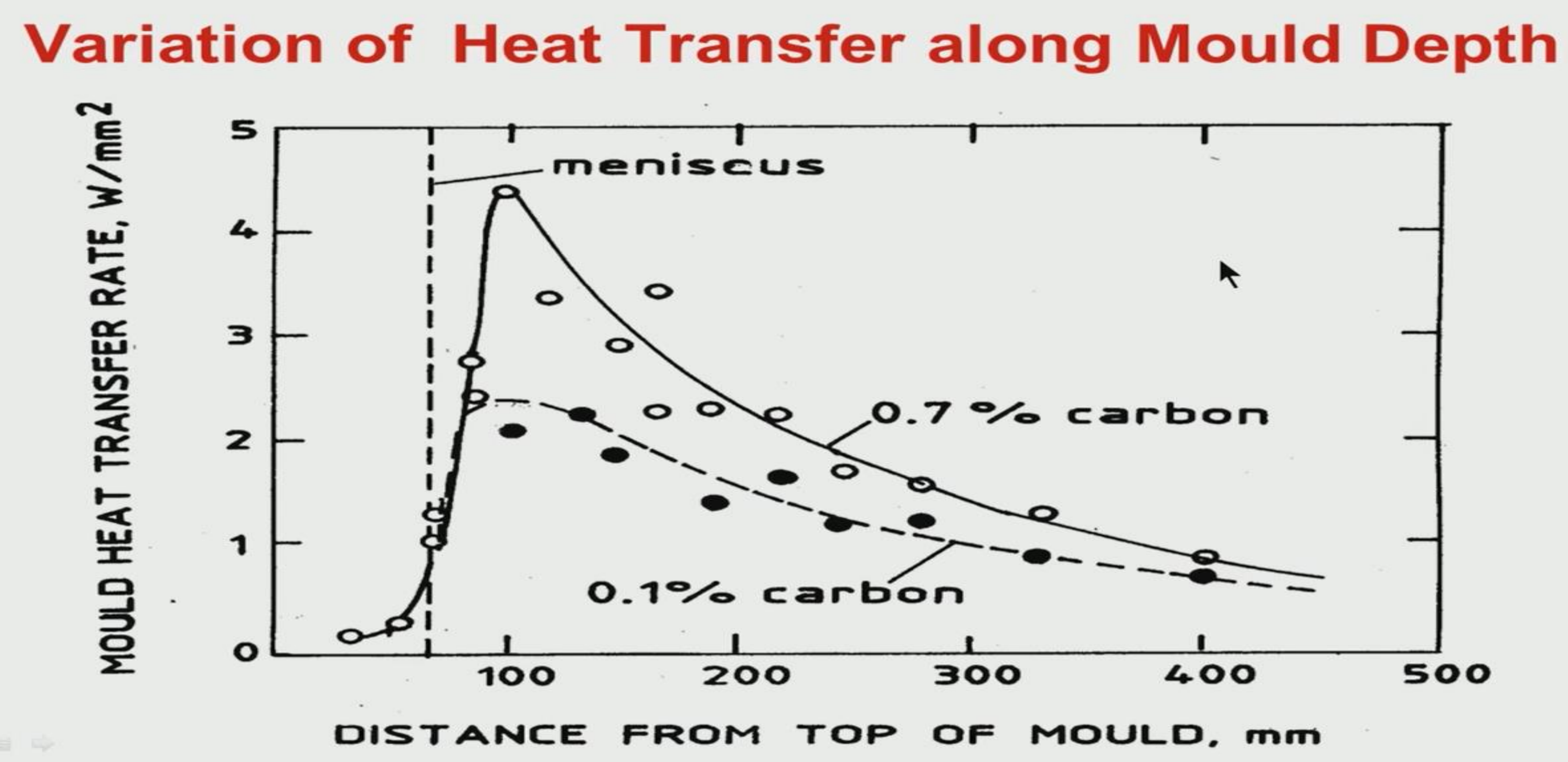
Case(c). Continuous:

The liquid and solid phases are fully dispersed throughout the phase change region and at the chosen scale there is no distinct interface between the solid and liquid phases; for example the solidification of wax, polymers or glasses.

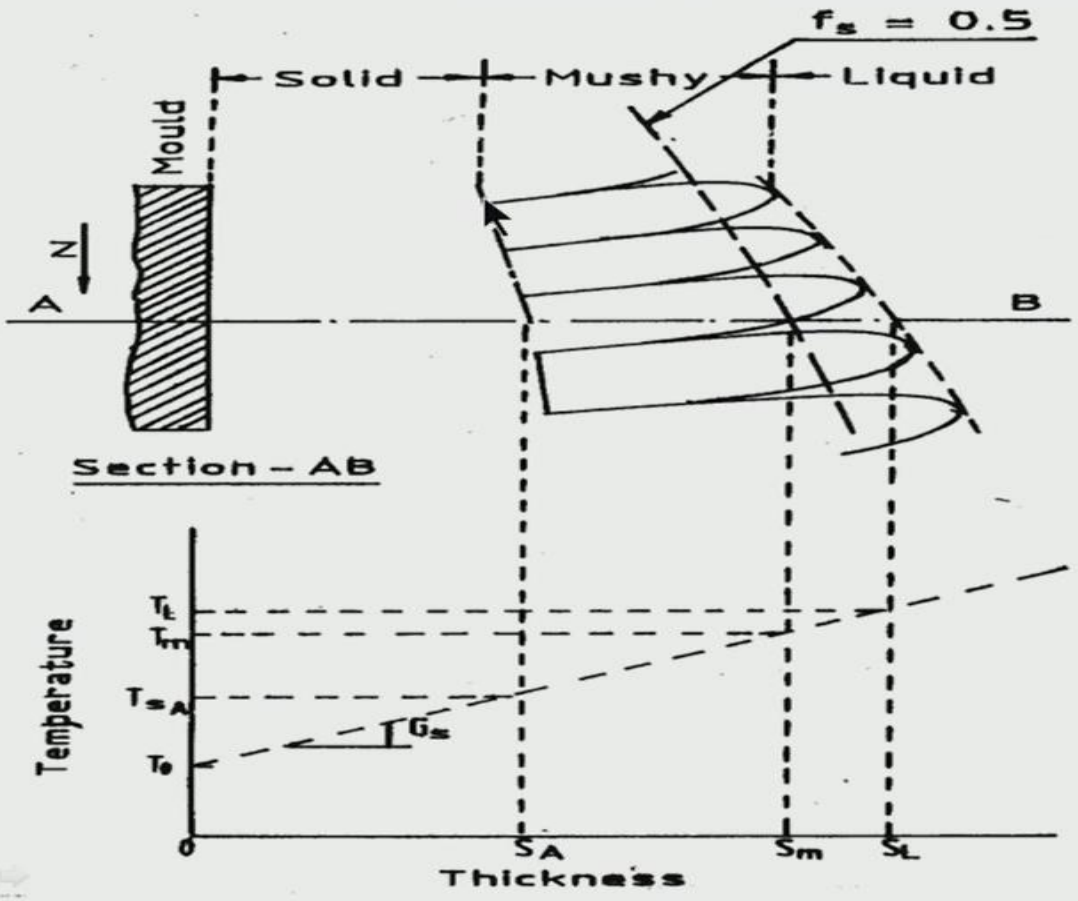
How heat is extracted from molten steel to the mold



How heat is extracted from molten steel to the mold



Temperature and Thickness Corresponding to Solid - Liquid Region



f_s : Solid fraction
T_o : Strand surface temp.
T_L : Liquidus temp.
T_m : Temp. f_s = 0.5
T_{sA} : Actual solidus temp.
S_A : Actual thickness of solid
S_m : Thickness at f_s = 0.5
S_L : Thickness at f_s = 0
G_s : Temp. gradient in shell

Solid Shell Thickness related to $(T_{SA} - T_O)$

Mushy Zone Depth related to $(T_L - T_{SA})$

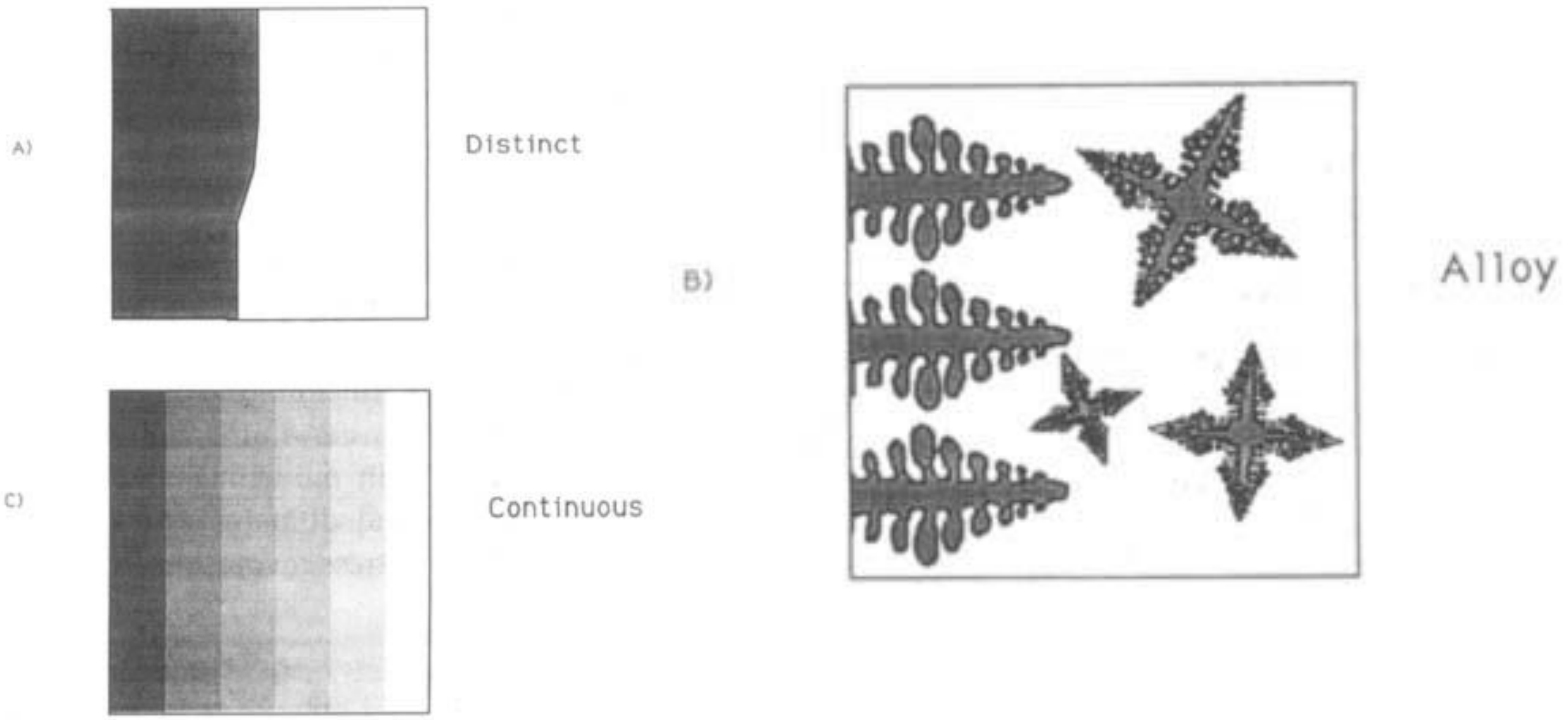


Figure 1 phase change types

Classification of phase change types

- In a distinct phase change, case (a), the state of the system is conveniently characterized by the position of the interface. In such cases the class of so called ‘front tracking’ methods’ offer an alternative solution approach to fixed grid methods.

- However, as the solid/liquid interface becomes less distinct (cases (b) and (c)), front tracking becomes computationally expensive if not impossible. In such cases, we feel that characterization of the phase change is best achieved by a model based on the phase fractions. Further, models of this nature are more easily numerically implemented using a fixed grid method.

Assignment/reading/submission

- What are PCMs(Phase change materials)?
- Discuss the theoretical and Numerical modeling aspects of PCMs for thermal Energy storage application.
- What physical phenomena and mechanism differ PCMs from conventional energy storage systems such as “pebble beds”?

Solving techniques

The release or absorption of the latent heat of fusion at the solid-liquid interface is generally solved using two methods;

I. Fixed mesh
II. Moving mesh

Fixed mesh

Fixed mesh involves the solution of a continuous system with an implicit(absolute) representation of the phase change.

Moving mesh

Moving mesh (Front tracking); the solid-liquid regions are treated separately and the phase change interface is explicitly(clearly) determined as a moving boundary.

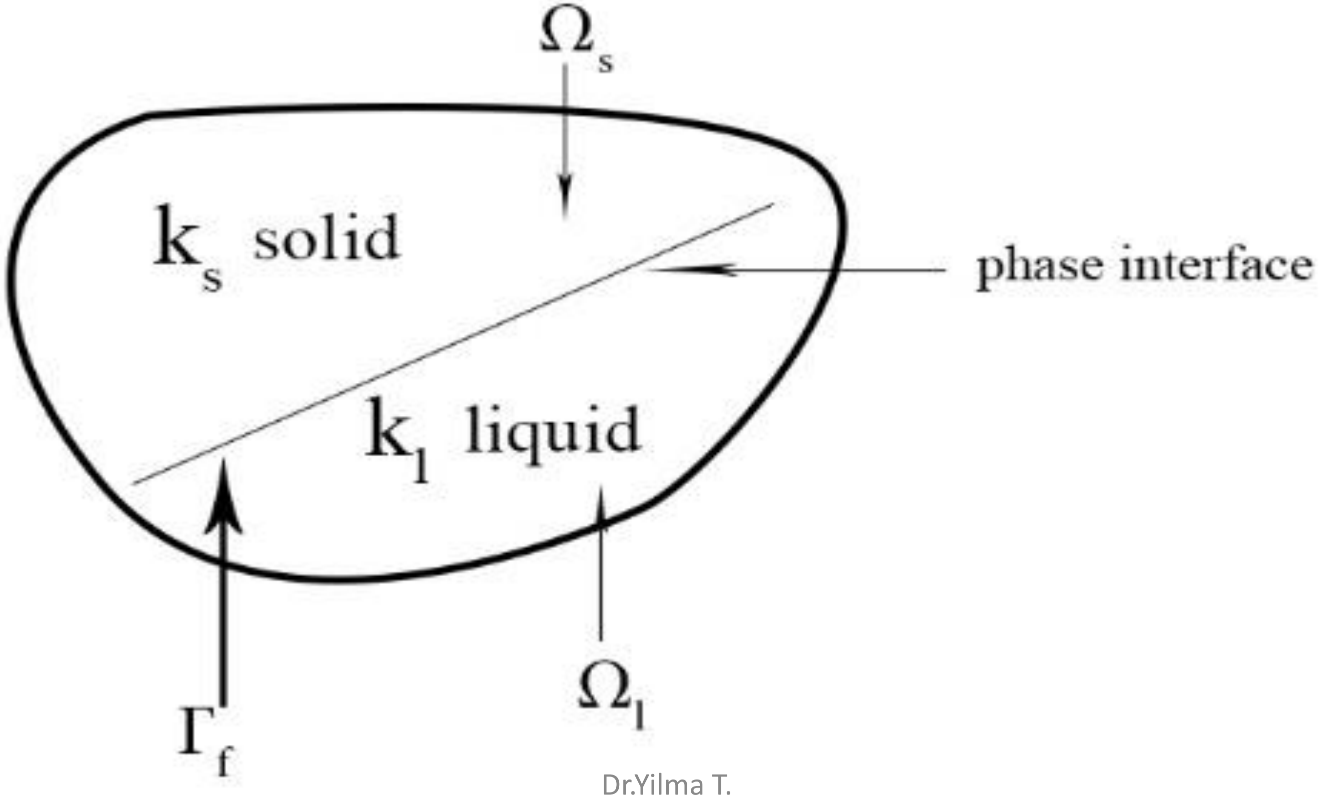
Moving mesh cont..

- The temperature at which the phase transition occurs is the melting point.
- The ‘enthalpy’ of fusion is a latent heat because during melting, the introduction of heat cannot be observed as a temperature change because the temperature is constant during the process.

Modeling of phase change process

Considering conservation of energy in the domain by dividing two distinct domains Ω_l and Ω_s ,

where $\Omega_l + \Omega_s = \Omega$. The energy conservation is written for one-dimensional case



Modeling cont..

$$\rho_l c_l \frac{\partial T}{\partial t} = k_l \frac{\partial^2 T}{\partial x^2} \text{ In } \Omega_l \text{ .... } (1)$$

$$\rho_s c_s \frac{\partial T}{\partial t} = k_s \frac{\partial^2 T}{\partial x^2} \text{ In } \Omega_s \text{ .... } (2)$$

Where *l* and *s* denote liquid and solid, respectively.

Modeling cont..

- The complete description of the problem involves the interface condition on phase change boundary, Γs, which are

$$T_{sl} = T_f$$

$$-k_s\left(\frac{\partial T}{\partial x}\right)_s = \rho_s Q_l \frac{ds}{dt} - k_l\left(\frac{\partial T}{\partial x}\right)_l \text{ On } \Gamma_{sl} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Where s represents the position of the interface, $\frac{ds}{dt}$ the interface velocity and T_f is the phase change temperature, Q_L = latent heat of fusion.

Modeling cont..

- *Equation (3) states that the heat transferred by conduction in the solidified portion is equal to the heat entering the interface by latent heat liberation at the interface and the heat coming from the liquid by conduction*.
- At the interface, there will be a jump abruptly, and then discontinuous problems will appear.

Numerical Methods for Modeling Phase Change

Enthalpy method (Fixed grid method)

- Offer a more general solution since they account for the phase change condition implicitly without attempting a priori to establish the position of the front.
- A single energy conservation equation is written for the whole domain as

$$\frac{\partial H}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \text{ In } \Omega \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3.1)$$

Numerical methods cont..

- Where H is the enthalpy function or the total heat content which is defined for isothermal phase change as

$$H(T) = \int_{T_r}^{T} \rho c_s(T)dT \text{ ....} T \leq T_f \text{ ....} \quad (3.2)$$

$$H(T) = \int_{T_r}^{T_f} \rho c_s(T)dT + \rho Q_L + \int_{T_f}^{T} \rho c_l(T)dT \text{ ....} T \geq T_l \text{ ....} \quad (3.3)$$

Numerical methods cont..

- For the phase change over an interval of temperatures of T_s and T_l,

which are the solidus and the liquidus, respectively, we have

$$H(T) = \int_{T_r}^{T_s} \rho c_s(T)dT + \rho Q_L + \int_{T_s}^{T} \left[\rho \frac{dQ_L}{dT} + \rho c_f(T) \right] dT \text{ ....} \left(T_s < T \le T_l\right) \text{ .... (3.4)}$$

$$H(T) = \int_{T_r}^{T_s} \rho c_s(T)dT + \rho Q_L + \int_{T_f}^{T_l} \rho c_f(T)dT + \int_{T_l}^{T} \rho c_l(T)dT \text{ ....} \left(T \ge T_l\right) \text{ .... (3.5)}$$

- Where c_f is the specific heat in the freezing interval
- Q_L is the latent heat
- T_r is the reference temperature below Ts

Numerical methods cont..

- Among the fixed mesh methods, one of the most commonly used methods has been the "effective heat capacity" method. This method is derived from writing

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \text{ In } \Omega \text{.......................................} \quad (3.6)$$

We can write

$$C_{eff} = \frac{dH}{dT} \quad \text{(From the standard heat conduction equation)}$$

Where ceff is the effective heat capacity. From equation (3.5), we can see that

Numerical methods cont..

$$c_{eff} = \rho c_s \text{ .... } (T<T_s)$$

$$c_{eff} = \rho c_f + \frac{Q_L}{T_R - T_S} \text{ .... } (T_s<T<T_l)$$

$$c_{eff} = \rho c_l \text{ .... } (T>T_l)$$

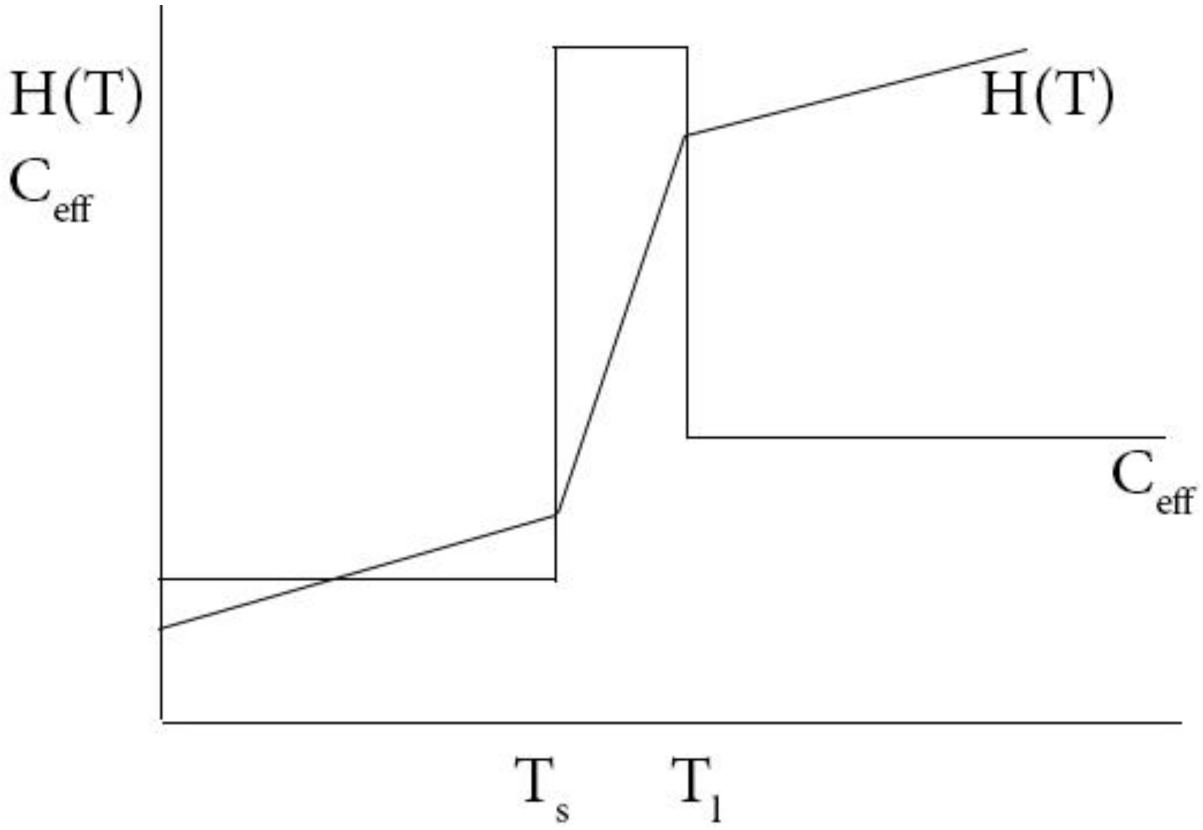


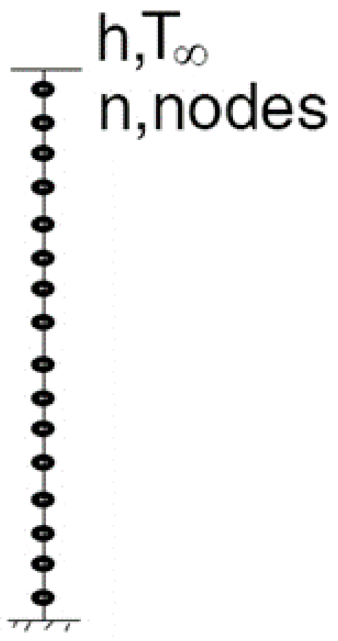
Fig. 3 Typical variation of enthalpy & c_{eff} with temperature

Numerical methods cont..

- To use “directly evaluated effective heat capacity” method, it will be necessary to maintain an interval of temperature for the evolution of latent heat, otherwise the effective heat capacity will be infinite.
- From this figure, we can see that effective heat capacity method can’t model isothermal phase change due to the requirement of a temperature change ($T_s \rightarrow T_R$).
- Thus, the enthalpy method corrects this, which is by defining the heat capacity as a smooth function of temperature.
- In fixed mesh technique, properties are interpolated using nodal temperature at every time step.
- The phase interface is calculated at every time step.

Numerical methods cont..

- Examples: Freezing of Sea
- One dimensional FDM for both melting and solidifying
- Modeling and GE discretization



- Heat conduction can be assumed with $\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}$ (one dimensional)
- Velocities in the liquid are so small and we can neglect the convection effect
- When the water reaches $0^{\circ}C$, it starts to freeze.

At the boundary nodes

$$-k\frac{(T_1 - T_2)}{\Delta x} = h(T_1 - T_\infty)$$

$$T_1 - T_2 = \frac{\Delta x h}{k}(T_1 - T_\infty)$$

$$T_1 = \frac{T_\infty}{(1+\frac{\Delta x h}{k})} + T_2$$

For interior node (using forward explicit method)

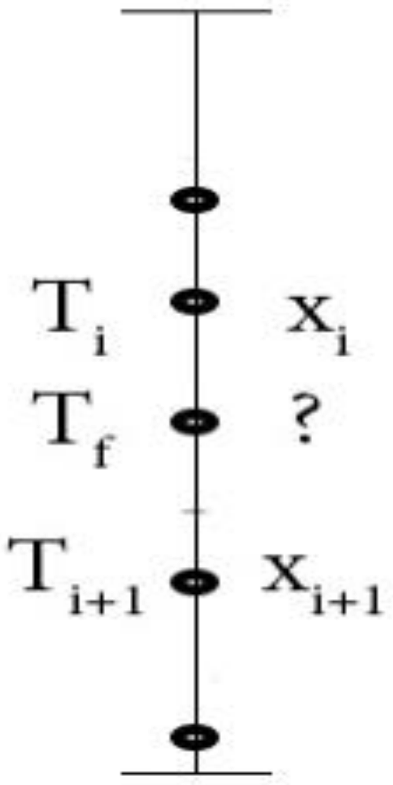
$$\rho c \frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{T_{i+1}{}^n - 2T_i^n - T_{i-1}{}^n}{\Delta x^2}$$ From 2 to n-1

$$T_i^{n+1} = T_i^n + \frac{k\Delta t}{\rho c \Delta x^2}\left(T_{i+1}{}^n - 2T_i^n - T_{i-1}{}^n\right)$$

For the last node (insulated),

$$-k\frac{(T_n - T_{n-1})}{\Delta x} = 0$$

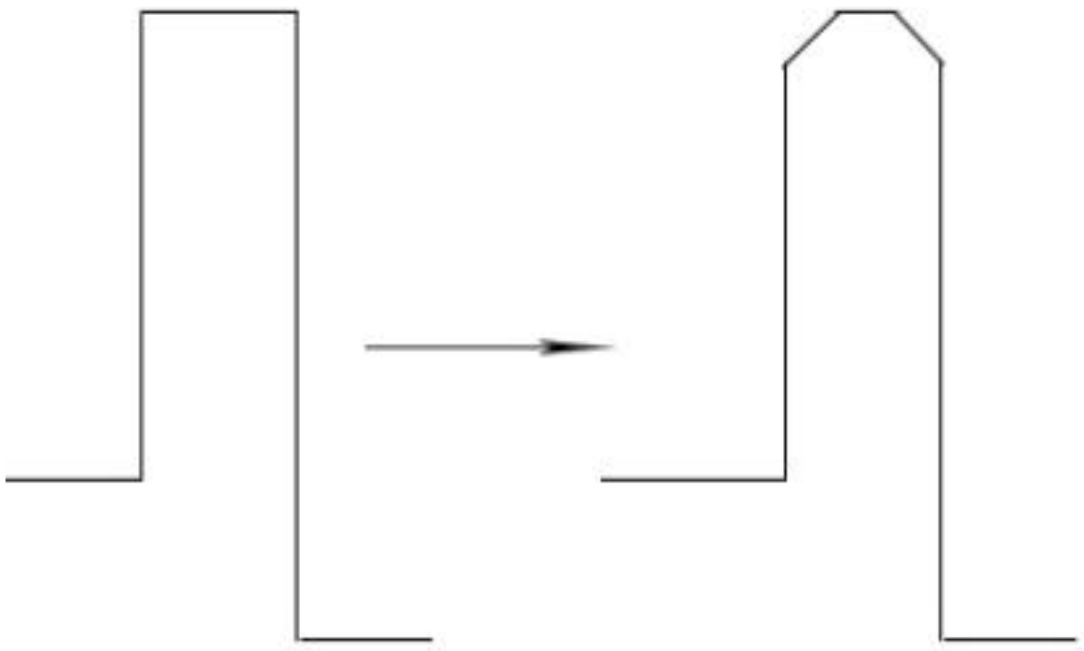
$$T_n = T_{n-1}$$



Interpolation: $x = x_i + \dfrac{T_f - T_2}{T_{i+1} - T_i}\left(x_{i+1} - x_i\right)$

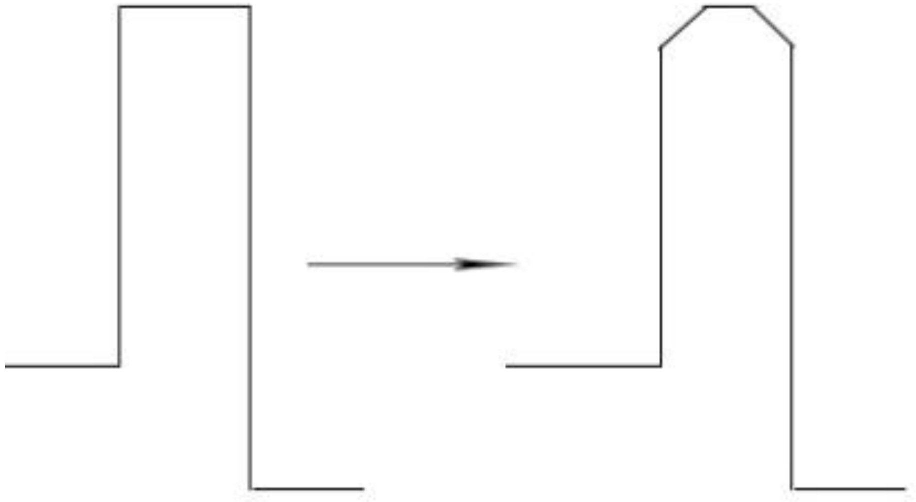
Algorithm

1. Discretize the domain with equidistant mesh
2. Calculate the fictitious specific heat to account for the latent heat and store data for interpolation in vector
    - **T** **c**
    - T_1 c_{s1}
    - T_2 c_{s2}
    - $T_{f-0.11}$ c_{s3}
    - $T_{f-0.1}$ c_f
    - $T_{f+0.1}$ c_l
    - $T_{f+0.11}$ c_{l2}
    - T_3 c_{l3}
    - T_4 c_{l4}



At T_f=finite temperature,

$$c_f = \frac{c_s + c_l}{2} + \frac{Q_L}{\Delta T} \leftrightarrow T_f = \frac{c_s + c_l}{2} + \frac{Q_L}{\Delta T}$$



- 3. Solutions by FDM
- 3.1 Surface Node

$$-k\frac{(T_1-T_2)}{\Delta x}=h(T_1-T_\infty)$$

$$T_1(h\Delta x+k)=\Delta xhT_\infty+kT_2$$

$$T_1=\frac{\Delta xhT_\infty+kT_2}{h\Delta x+k}$$

3.2 Interior Node

- from 2 to m-1

$$T_i^{n+1} = T_i^n + \frac{k\Delta t}{\rho c}\left(\frac{T_{i+1}{}^n - 2T_i^n - T_{i-1}{}^n}{\Delta x^2}\right)$$

- 3.3 End Node

$$T_m = T_{m-1}$$

because the end of the water is ground which is an insulated type of boundary condition

$$-k\frac{(T_m - T_{m-1})}{\Delta x} = 0$$

3.4 Phase Interface

$$x_t = x_i + \frac{T_f - T_2}{T_{i+1} - T_i}\left(x_{i+1} - x_i\right)$$

3.5 if ($t<t_{max}$)

$$t \leftarrow t + \Delta t$$

Repeat from 3.1.

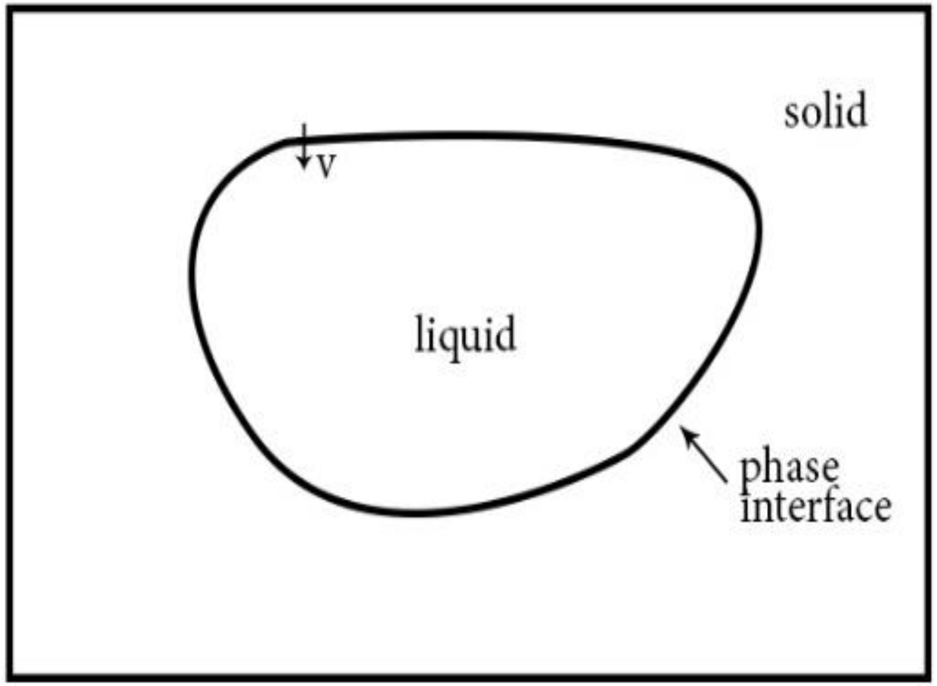
Moving mesh techniques

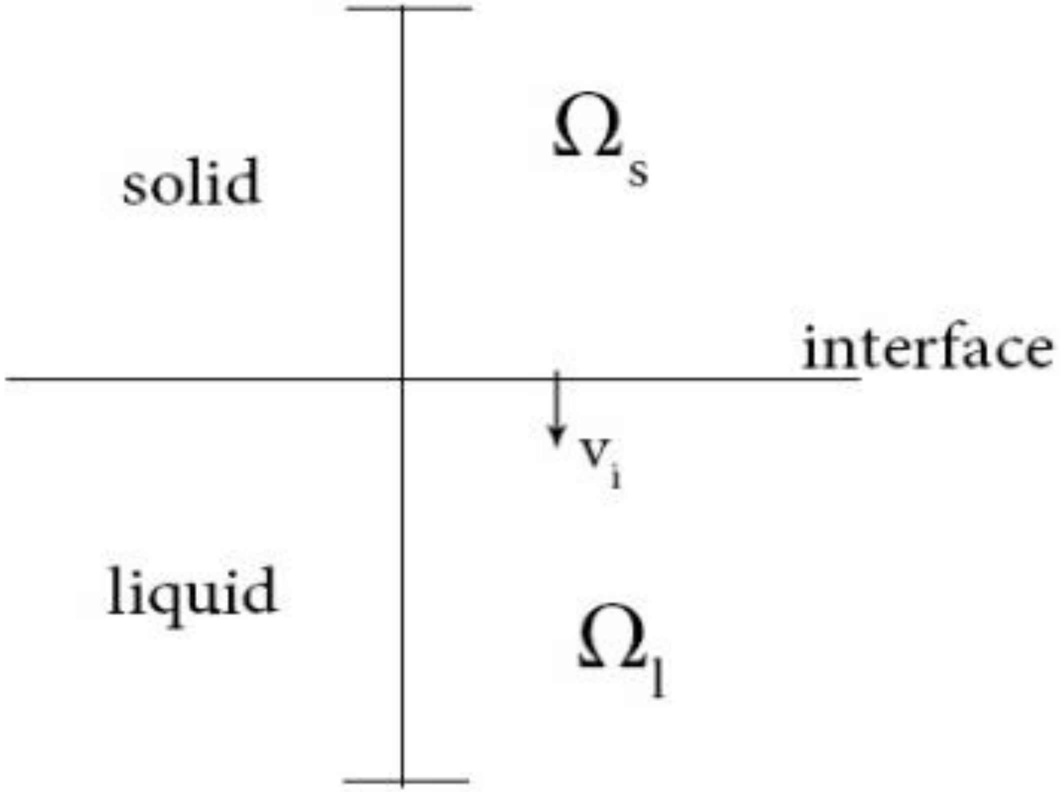
- A boundary separating two different phases which develops in a phase change problem moves in the matter during the process. Transport properties vary considerably between phases, which result in totally different rates of energy, mass and momentum transport from one phase to another. In these problems, the position of the moving boundary cannot be identified in advance, but has to be determined as an important constituent of the solution.
- The term ‘moving boundary problems’ is associated with time-dependent boundary problems, where the position of the moving boundary must be determined as a function of time and space.
- Moving boundary problems, also referred to as Stefan problems, were studied as early as 1831 by Lame and Clapeyron [1].

Moving mesh techniques

1. Use FEM because it has two domains
2. Use transient non-linear heat transfer
3. For casting problems, use fixed mesh technique and adopt to moving mesh

Physical model





Governing equations

1. $\rho_s c_s \dfrac{\partial T}{\partial t} = k_s \dfrac{\partial^2 T}{\partial x^2}$ in Ω_s ....Eq(1)

2. $\rho_l c_l \dfrac{\partial T}{\partial t} = k_l \dfrac{\partial^2 T}{\partial x^2}$ in Ω_l ....Eq(2)

3. At the interface

$$T = T_f$$

GE's cont..

$$k\left(\frac{\partial T}{\partial x}\right)_l - k\left(\frac{\partial T}{\partial x}\right)_s = \rho Q_L \frac{dx_i}{dt}$$

$$k_l\left(\frac{\partial T}{\partial x}\right)_l - k_s\left(\frac{\partial T}{\partial x}\right)_s = \rho Q_L \frac{dx_i}{dt} \quad \text{.............} \text{ (a)}$$

$$-k_l \frac{\partial T}{\partial x} = -k_l \frac{T_i - T_{i+1}}{\Delta x}$$

$$-k_s \frac{\partial T}{\partial x} = -k_s \frac{T_i - T_{i-1}}{\Delta x}$$

Cont..

$V * \Delta t = \Delta x$, where V is the velocity of the interface and △x is the mesh displacement.

Thus, substituting

$$-k_l \frac{T_i - T_{i+1}}{\Delta x} + -k_s \frac{T_i - T_{i-1}}{\Delta x} = \rho Q_L \frac{dx_i}{dt} \quad \text{.............} \text{(b)}$$

$$v_{\text{int}} = \frac{dxi}{dt} = \frac{\dfrac{-k_l(T_i - T_{i+1})}{\Delta x} - \dfrac{-k_s(T_i - T_{i-1})}{\Delta x}}{\rho Q_L}$$

Cont..

- V_{int} is the velocity of the interface

$\rho A \Delta x_i Q_L$ - Heat rejected by the liquid where freezing

$\rho A \Delta x_i$ is $\dot{m}$ and Q_L is the latent heat of fusion.

Modifying the PDEs For Moving Mesh Method

- We use

$$\frac{\Delta T}{\Delta t} = \frac{\partial x}{\partial t}\frac{\partial T}{\partial x} + \frac{\partial T}{\partial t}$$

  - x is changing with time

  This is from material derivative

Cont..

$$\frac{D(...)}{Dt} = \frac{\partial(...)}{\partial t} + V \cdot \nabla(...)$$, Where in the (...), the property will be put

Thus, $$\frac{\Delta T}{\Delta t} = \frac{\partial T}{\partial t} + \frac{\partial x}{\partial t}\left(\frac{\partial T}{\partial x}\right)$$

Now, equation (1) becomes

$$\rho_s c_s \left(\frac{\partial x}{\partial t}\frac{\partial T}{\partial x} + \frac{\partial T}{\partial t} \right) = k_s \frac{\partial^2 T}{\partial x^2} \text{ .... } (3)$$

Cont..

- Equation (2) becomes

$$\rho_l c_l \left(\frac{\partial x}{\partial t} \frac{\partial T}{\partial x} + \frac{\partial T}{\partial t} \right) = k_l \frac{\partial^2 T}{\partial x^2} \quad \ldots\ldots\ldots\ldots\ldots (4)$$

From Equation (3), for the solid part

Cont..

$$\frac{\partial T}{\partial t} = \frac{k_s}{\rho_s c_s}\frac{\partial^2 T}{\partial x^2} - v\frac{\partial T}{\partial x}$$

$$\frac{T_i^{n+1} - T_i^{n}}{\Delta t} = \frac{k_s}{\rho_s c_s}\left(\frac{T_{i+1}{}^{n} - 2T_i^{n} + T_{i-1}{}^{n}}{(\Delta x)^2}\right) - v_i\left(\frac{T_{i+1}{}^{n} - T_{i-1}{}^{n}}{2\Delta x}\right)$$

$$T_i^{n+1} = T_i^{n} + \frac{\Delta t k_s}{\rho_s c_s}\left(\frac{T_{i+1}{}^{n} - 2T_i^{n} + T_{i-1}{}^{n}}{(\Delta x)^2}\right) - \Delta t v_i\left(\frac{T_{i+1}{}^{n} - T_{i-1}{}^{n}}{2\Delta x}\right)$$

For the liquid

$$T_i^{n+1} = T_i^{\,n} + \frac{\Delta t k_l}{\rho_l c_l}\left(\frac{T_{i+1}{}^{n} - 2T_i{}^{n} + T_{i-1}{}^{n}}{(\Delta x)^2}\right) - \Delta t v_i\left(\frac{T_{i+1}{}^{n} - T_{i-1}{}^{n}}{2\Delta x}\right)$$

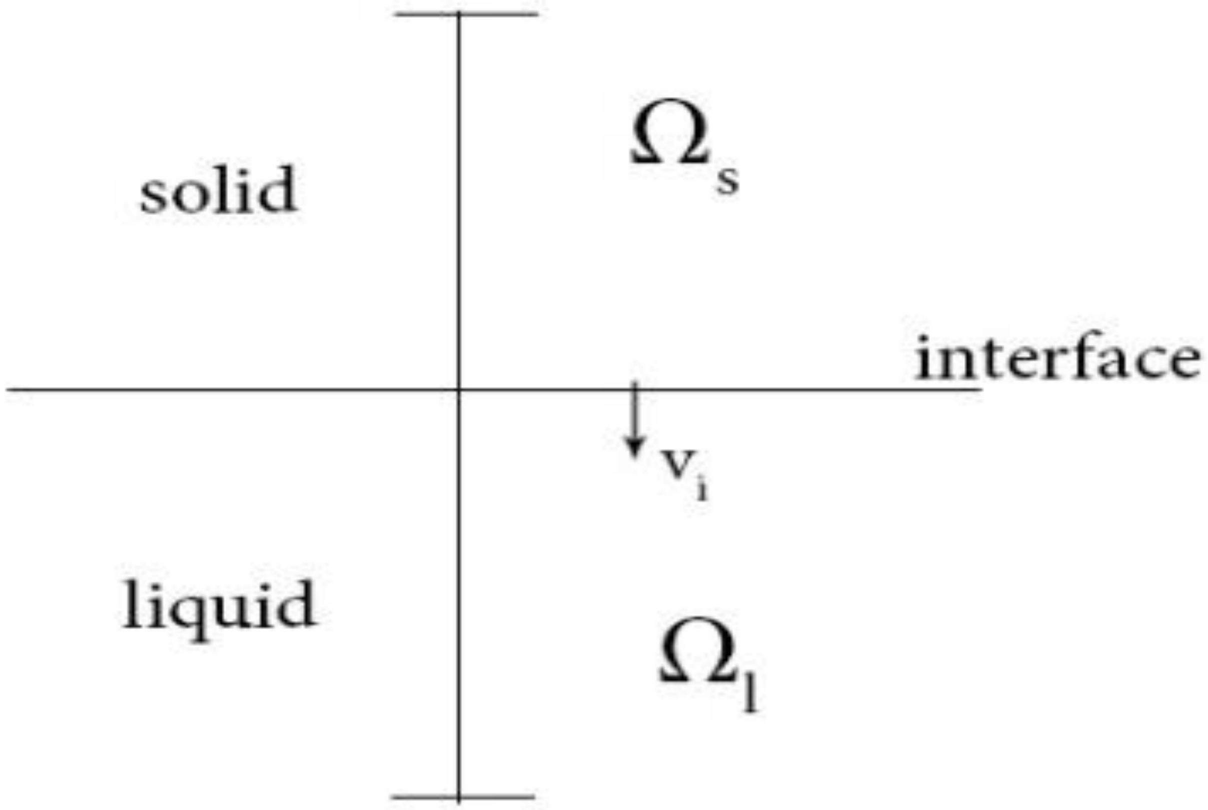
Mesh Velocity

For the solid

At x_i=0, v_i =0

$$v_{mesh} = v_{\text{int}\,er}\left(\frac{x_i}{x_{\text{int}\,erface}}\right)$$

Cont..



For the liquid

- At $x_i=x_{interface}$, $v_m=v_{interface}$ and At $x_i=x_m$, $v_m=0$.

$$v_{mesh} = v_{\text{interface}}\left(\frac{x_m - x_i}{x_m - x_{\text{interface}}}\right)$$

where

$$\mathrm{V}_{\mathrm{interface}} = \frac{\dfrac{-\mathrm{k}_l(\mathrm{T}_i - \mathrm{T}_{i+1})}{\Delta x} - \dfrac{-k_s(T_i - T_{i-1})}{\Delta x}}{\rho Q_L}$$

Boundary Condition

1. Convective Boundary Condition

$$\frac{-k_s(T_1 - T_2)}{\Delta x} = h(T_1 - T_\infty)$$

$$T_1 = \frac{h\Delta x T_\infty + k_s T_2}{(h\Delta x + k)}$$

2. Interface

$$T_{\text{int}} = T_f$$

3. Insulated

$$T_m = T_{m-1}$$

Update mesh movement

$x_i^{n+1} = x_i^n + v_i \Delta t$ for i=1 to n+1

Algorithm for moving mesh

1. Input geometry and thermo-physical properties
2. Assume infinitesimal frozen (melted) layer
3. Divide the liquid and solid domains to equal number of mesh each greater than 10 and generate node coordinates
4. Initialize time counter
5. Solve at each time step

Algorithm cont..

5.1. Impose boundary conditions

$$T_1 = \frac{h\Delta x T_\infty + k_s T_2}{(h\Delta x + k)}$$

5.2. $T_k = T_f$ for 1→k - solid

k→m - liquid

5.3. Mesh velocity

$$\mathrm{V_m} = \frac{-\mathrm{k_s}(\mathrm{T_k} - \mathrm{T_{k+1}}) - k_l(T_k - T_{k-1})}{\Delta x \rho Q_L}$$

$$v_i = v_m \frac{x}{x_k} \quad \text{i≤k}$$

$$v_i = v_m \frac{x - x_k}{x_m - x_k} \quad \text{for i→k-m}$$

Algorithm cont..

$Q_s = Q_l + Q_L$ Where Q_s is the heat to the solid

Q_l Is the heat to the liquid and Q_L is the latent heat of fusion

5.4. For i=2 to m-1 and i≠k

$$T_i^{n+1} = T_i^n + \frac{\Delta t k}{\rho c}\left(\frac{T_{i+1}{}^n - 2T_i^n + T_{i-1}{}^n}{(\Delta x)^2}\right) - \Delta t v_i\left(\frac{T_{i+1}{}^n - T_{i-1}{}^n}{2\Delta x}\right)$$

For i<k→k=k_s

For i>k→k=k_l

5.5. $T_m = T_{m-1}$

5.6. if t<t_{max} repeat from 5.1.

Else

End