Thermal energy storage and thermal management using PCMs: heat transfer enhancement and advanced modelling

Part II

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Solidification - examples

Geometries:
• Cylindrical shells (tubes)
• Spherical shells

Features:
• Time to complete the process
• Instant melt fractions and heat fluxes
• Shrinkage and void formation

Objective:
• Generalization
• Void prediction
• Supercooling modeling
Cylindrical shell: cooling direction

Shamsundar and Sparrow (1976)

Experimental

Adiabatic bottom

Cooled bottom

Model

Liquid

Shell

Air

H

H*

Spherical shell: Modeling

• In the literature, the shell is initially filled with the liquid completely

• This leads to “concentric” solidification

• In reality, a completely filled shell is hardly possible
Solidification in a spherical shell

- $C=10^5$ gives results that do not fit the experiment
- However, $C=10^8$ gives good agreement with the experiment

Spherical shell: shrinkage and voids

- Yotvat and Zelikover (2008)
- Revankar and Croy (2007)
Generalization

Melt fraction vs. FoSte

Solidification: connected volume, no voids

Absence of voids means high reliability and repeatability

The solidification process is used in various procedures such as thermal energy storage, organ preservation and food storage.

Some phase change materials (PCMs) are exposed to the subcooling phenomenon.

Solidification in the presence of subcooling is unexpected and sometimes unwanted.

Today, only a small amount of models take the subcooling phenomenon into account.

This study includes the development of a numerical model validated against experimental work.

What is Subcooling?

Solidification **without** subcooling

1. Liquid
2. Solidification
3. Solid

Solidification **with** subcooling

1. Liquid
2. Subcooled liquid
3. Solidification
4. Solid

Enthalpy and Temperature

- Rapid solidification
- Adiabatic process
- Constant system enthalpy
- Latent heat is used to raise the PCM’s temperature
- The ratio between solid and liquid is in accordance to the enthalpy

M.E. Glicksman (2001) Principles of Solidification
Experimental studies

- A great deal of experimental studies dating as early as 1949.
- Known effects of four major parameters on the degree of subcooling:
  - $\uparrow$ Volume - Degree of subcooling $\downarrow$
    - Bigg (1953), Chen et al. (1999)
  - $\uparrow$ Cooling rate - Degree of subcooling $\uparrow$
    - Chen and Lee (1998), Yoon et al. (2001)
  - $\uparrow$ Surface roughness - Degree of subcooling $\downarrow$
    - Saito et al. (1990), Okawa et al. (2002)
  - $\uparrow$ Nucleation agent mass - Degree of subcooling $\downarrow$
    - Hozumi et al. (2002), Liu et al. (2015)

Subcooling Models

- Bédécarrats et al. (1996) Phase-change thermal energy storage using spherical capsules performance of a test plant
- Le Bot and Delaunay (2008) Rapid solidification of indium: modeling subcooling
- Kousksou et al. (2010) Forced convection heat transfer in supercooled phase change material suspensions with stochastic crystallization
- Font et al. (2013) One dimensional solidification of supercooled melts
Subcooling Models

- Günther et al. (2007) Modeling of subcooling and solidification of phase change materials

Basics of the current model

Enthalpy-Temperature relation

\[
h(T) = c_p(T - T_m) + \frac{L}{2} \text{erf}\left(\frac{T - T_m}{\delta T}\right)
\]

\[
h(T) = \begin{cases} 
  c_p(T - T_m) - 0.5L & \text{(Solid)} \\
  c_p(T - T_m) + 0.5L & \text{(Liquid)} 
\end{cases}
\]
Basics of the current model
Phase change

\[ p = 0 \quad \text{Liquid} \]
\[ p = 1 \quad \text{Solid} \]
\[ p = 2 \quad \text{Phase change} \]

\[ \phi^{n+1} = \phi^n + \frac{\Delta f}{\Delta x} V \]
\[ T^{n+1} = \phi T_s + (1 - \phi) T_i \]

“Solidification speed”

In the present study, the relation discussed by Ashby and Jones (2006) is applied:

\[ V = \frac{d}{6h_p} \exp \left( \frac{-\Delta G_a}{k_B T_m} \right) \frac{L(T_m - T)}{T_m} \]

where \( d \) is the molecular diameter of the specific phase-change material, \( h_p \) is Planck's constant, \( \Delta G_a \) is the activation energy and \( k_B \) is Boltzmann's constant. After calculating the value of \( \phi \), one can assess the new temperature as:

\[ T = \frac{\phi}{\phi_{\text{max}}} T(Solidification) + \left( 1 - \frac{\phi}{\phi_{\text{max}}} \right) T(Liquid) \]
Basics of the current model
Discrete energy equation

\[ \frac{\rho \partial h}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \]

\[ h_{i+1}^{n+1} = h_i^n + \frac{\Delta t}{\rho \Delta x} \left[ \frac{T_{i+1}^n - T_{i}^n}{R_{h+}} - \frac{T_{i}^n - T_{i-1}^n}{R_{h-}} \right] \quad i = 2 \ldots N-1 \]

\[ T_{i+1}^{n+1} = \begin{cases} T_m + \frac{h_{i+1}^{n+1} + 0.5L}{c_p} & \text{(Solid)} \\ T_m + \frac{h_{i+1}^{n+1} - 0.5L}{c_p} & \text{(Liquid)} \end{cases} \]

Further development
One dimensional cylindrical model

- One dimensional cylindrical system
- Heat transfer is limited to conduction in the radial direction alone
- No heat can go through the cylindrical center
- Cylindrical wall is kept at a constant temperature
- No density change due to phase change
Further development
One dimensional cylindrical model

\[ \hat{r} \quad 1 \quad 2 \quad \Delta r \quad N \]

\[ q_i \cdot \frac{T_i - T_{i-1}}{\Delta r} = 0 \]
\[ \bar{T}_i = \bar{T}_{i-1} \]

\[ h_i^{n+1} = h_i^n + \frac{4}{3} \rho \Delta r \cdot k_i (\bar{T}_i^n - T_i^n) \]
\[ h_i^{n+1} = h_i^n + \frac{\Delta t}{\rho (i - 0.5) \Delta r} \left[ k_{i+0.5} (T_{i+0.5}^n - T_i^n) - (i - 1) k_{i-0.5} (T_i^n - T_{i-1}^n) \right] \]

Single phase, 1D Validation

<table>
<thead>
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<th>Property</th>
<th>Units</th>
<th>Value</th>
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<tr>
<td>( k )</td>
<td>( \text{W/m}^\circ C )</td>
<td>0.654</td>
</tr>
<tr>
<td>( c_p )</td>
<td>( \text{kJ/kg}^\circ C )</td>
<td>4.179</td>
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<tr>
<td>( \rho )</td>
<td>( \text{kg/m}^3 )</td>
<td>983.3</td>
</tr>
<tr>
<td>( \mu )</td>
<td>( \text{m/s} )</td>
<td>1.59 \times 10^{-5}</td>
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<tr>
<td>( T_{\text{init}} )</td>
<td>( ^\circ C )</td>
<td>5</td>
</tr>
<tr>
<td>( T_{\text{wall}} )</td>
<td>( ^\circ C )</td>
<td>60</td>
</tr>
<tr>
<td>( R )</td>
<td>( \text{m} )</td>
<td>0.025</td>
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</table>

\[ T(r,t) = T_{\text{wall}} + \frac{2(T_{\text{wall}} - T_{\text{init}})}{R} \sum_{n=1} J_0 \left( \omega_n r \right) \frac{e^{-\alpha_n^2 t}}{\omega_n J_1(\omega_n R)} \]
Two dimensional model

\[ \rho \frac{\partial h}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \]

\[ h_{ij}^{n+1} = h_{ij}^{n} + \frac{\Delta t}{2 \rho_{ij} \Delta r^2} \left[ \zeta_{1} T_{i+1,j}^{n} + \zeta_{2} T_{i-1,j}^{n} + \zeta_{3} T_{i,j+1}^{n} + \zeta_{4} T_{i,j-1}^{n} - (\zeta_{1} + \zeta_{2} + \zeta_{3} + \zeta_{4}) T_{ij}^{n} \right] \]

- Heat transfer is limited to conduction in the radial and axial directions
- No heat can go through the cylindrical center
- Cylindrical wall and base are kept at a constant temperature
- Top of the cylinder is kept insulated

Single phase, 2D Validation

\[ T(r, z, t) = T_{wall} + \frac{4(T_{wall} - T_{wall})}{HR} \sum_{n=0}^{\infty} \sum_{\omega_{n} = \omega_{0}}^{\infty} \frac{J_{0}(\omega_{n} r)}{\alpha_{n}} J_{1}(\omega_{n} R) \frac{\sin(\beta_{n} z)}{\beta_{n}} \exp\left[ -\alpha \left( \beta_{n}^2 + \omega_{n}^2 \right) t \right] \]
Solidification mold

\[ \rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \]

\[ T_{y+1} = T_y + \frac{\Delta t}{2 \rho_0 c_p \Delta r^2} \left[ \zeta_{ij} T_{ij} + \zeta_{2i} T_{ii+1} + \zeta_{3j} T_{ij+1} + \zeta_{4j} T_{i+1j} - (\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4) T_y \right] \]

Experiments
“Regular” solidification (expected)

- Anomalous materials like Ga and water - liquid density is larger than the solid density.

- If no density change during solidification.

Energy balance condition

- Energy balance:

\[ m_i L = m_s c_{pl} (T_s - T_n) + m_i c_{pl} (T_l - T_n) \]

\[ m_i = m_{total} - m_s \]

- Mass conservation:

\[ m_i = \frac{c_{pl} (T_l - T_n)}{L + c_{pl} (T_l - T_n) - c_{pl} (T_s - T_n)} \]

- Solid fraction:

\[ SF_{\text{max}} = \frac{1}{1 + \frac{L - c_{pl} (T_m - T_s)}{c_{pl} (T_m - T_n)}} \]

\[ m_i = m_{total} - m_s \]
Energy balance confirmation

Comparison with experiments
Regular solidification patterns (predicted)

- Physically meaningful solidification patterns
- Mushy regions may fill the entire volume

Closing remarks

- A two-dimensional solidification model, which takes into account the subcooling phenomenon, was developed.
- Single phase cooling compared to analytical solutions with excellent agreement.
- Lack of compatibility between heat transfer rates and solid growth rate lead to a new model for the kinetic stage of solidification.
- The agreement between the experiments and model predictions was fairly good, including physically acceptable solidification patterns.
- Some discrepancies are probably due to the properties.
Some additional topics

• Simplified modeling

• Multiple-PCM systems

• Cold storage packages