Modeling Convection during Melting of a Phase Change Material

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Sensible Heat Storage:
A heat storage system that uses a heat storage medium, and where the addition or removal of heat results in a change in temperature.

Thermochemical Storage:
Storage of energy is the result of a chemical reaction.

Latent Heat Storage:
The storage of energy is the result of the phase change (solid-liquid or solid-solid) of a phase change material (PCM). The process happening over a small temperature range.
Finite Elements can be used to help in the design of Latent Heat Energy Storage Systems (LHESS):
- Determination of the application-dependent size of the LHESS;
- Choice of geometry;
- Heat Transfer enhancement (fins for example);
- Etc ...

All neglected convection in the liquid melt.
Application

Solar Collector

Heat exchanger and PCM Storage Tank

Finned Pipe

Hot water to house

Cold water supply
Geometry Studied

2D Convection Dominated
The phase change material used in the validation study is **ideal Octadecane**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity</td>
<td>0.2 W/m·K</td>
</tr>
<tr>
<td>Density</td>
<td>800 kg/m³</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>0.008 Pa·s</td>
</tr>
<tr>
<td>Heat Capacity</td>
<td>1.25 kJ/kg·K</td>
</tr>
<tr>
<td>Enthalpy of Fusion</td>
<td>125 kJ/kg</td>
</tr>
<tr>
<td>Melting Temperature</td>
<td>303 K</td>
</tr>
</tbody>
</table>
Numerical Modeling

2D Convection Dominated
Governing Equations

- Navier-Stokes and energy equation:

\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \rho g \alpha (T - T_0)
\]

\[
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)
\]

\[
\rho C_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)
\]

- Boundary Conditions:

\[
T(x = 0, t > 0) = T_w
\]

\[
T(x = 0.1m, t > 0) = T_m
\]

- Energy balance at the melting interface \( \delta(x,y,t) \):

\[
- \rho_1 L \frac{d\delta(x,y,t)}{dt} = k_l \frac{\partial T_l(\delta,t)}{\partial x} = -\rho_1 L u_m
\]
Modeling in COMSOL

- Problem type: Transient thermal fluid*

- Model used: Laminar Flow
  Heat Transfer in a Liquid
  Transient Analysis

These models encompass:
  - Laminar flow driven by the body force
  - Heat transfer by conduction and convection
  - Modified using the Effective Heat Capacity Method and a properly defined viscosity over the entire temperature range.

- 2D Geometry

* The treatment of phase change renders the problem non-linear as well.
Modified $C_p$ Method

\[ C_p = \begin{cases} 
C_{p,s} & T < 303 \text{ K} \\
C_{p,m} & 313 \text{ K} < T < 313 + \Delta T_m \text{ K} \\
C_{p,l} & T > 313 + \Delta T_m \text{ K} 
\end{cases} \]

Where

\[ C_{p, m} = \frac{L_f}{(\Delta T_m)} \]

\[ C_{p, s} = \text{Solid phase } C_p = 1.25 \text{ kJ/kg} \]

\[ C_{p, l} = \text{Liquid phase } C_p = 1.25 \text{ kJ/kg} \]

\[ L = \text{Latent heat of fusion} = 125 \text{ kJ/kg} \]

\[ \Delta T_m = \text{Melting Temperature range} \]
Modified $C_p$

Numerically, the modified $C_p$ is incorporated in COMSOL using the piecewise function in the material properties.

A continuous second derivative is used.
The dynamic viscosity, was input as a piecewise, continuous, second derivative function centered about $T_m$.

It accounted for the viscosity of the liquid PCM in the melted region and forced the solid PCM to remain fixed by having a solid viscosity of $10^8$. 
Mesh

- 2D quadrilateral elements;
- 4096 elements were selected, average element size of \(2.44 \times 10^{-6} \text{ m}^2\), selected after a mesh convergence study;
- Element size provided convergence at a relatively low run time, simulations took on average 7 hours on an Intel dual core processor.
Results

2D Convection Dominated
Melting interface and velocity profile at 5,000s for $\Delta T_m = 1$ K

Convection Dominated Melting
Result vs Bertrand et al.

Melting interface at 5,000s for $\Delta T_m = 1$ K
Effect of Melting Temperature Range
Real Impact of Convection

Conduction

Melted Fraction = 20.8%

Conduction + Convection

Melted Fraction = 34.2%

At 5,000s for $\Delta T_m = 1$ K

The physical processes encountered during transient phase change heat transfer, coupled with conduction and convection, in a PCM can be modeled numerically using COMSOL Multiphysics;

The appearance and the behavior of the melting front can be simulated by:
- modifying the specific heat of the PCM to account for the increased amount of energy, in the form of latent heat of fusion, needed to melt the PCM over its melting temperature range.
- modeling the entire PCM as a liquid with a modified viscosity taking an extremely high value that forces the “solid” PCM to behave as a solid.

The simulation showed the impact the melting temperature range selected has on the overall convection driven phase change process.