

Modeling Convection during Melting of a Phase Change Material

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Abstract: COMSOL Multiphysics can be used to model a latent heat energy storage system (LHESS). However, past numerical studies have neglected natural convection heat transfer in the melted phase change material (PCM), resulting in an under prediction of the total heat transfer rate to the PCM under most circumstances. A 2D numerical study was performed in COMSOL Multiphysics (4.0a and 4.1) to simulate melting of a PCM including both conduction and convection heat transfer. The heat transfer in fluids and laminar flow physics interfaces were used. To model natural convection, the proper volume force was applied to the PCM. The dynamic viscosity was input as a piecewise, continuous second derivative, function that 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 . In the simulations, natural convection was observed as the melted PCM rose to the top of the container and began circulating, moving the solid-liquid interface. The results show the importance of accounting for natural convection during melting in a PCM.

Keywords: Phase Change Heat Transfer, Melting, Natural Convection, Phase Change Material, Latent heat.

Nomenclature:

A_{tot}	Area of square PCM (m^2)
C_p	Specific heat capacity ($J/kg \cdot K$)
C_{pm}	Modified heat capacity ($J/kg \cdot K$)
F	Volume force (N)
g	Gravity (m/s^2)
L_f	Latent heat of fusion (kJ/kg)
MF	Melted fraction
T	Temperature (K)
T_o	Initial temperature (K)
T_m	Melting temperature (K)
T_w	Temperature of left wall (K)
t	Time (s)
α	Thermal expansion Coefficient ($1/K$)
ρ	Density (kg/m^3)
ν	Dynamic Viscosity ($Pa \cdot s$)

1. Introduction

Phase change materials (PCMs), used inside latent heat energy storage systems (LHESS) can be used to store thermal energy for various applications including: temperature control of photovoltaic cells and electronic components, climate control of building, etc. One of the most interesting applications is thermal energy storage in the form of latent heat for solar domestic hot water (SDHW) systems, reducing the space and weight requirements of the system [1]. In such case, the LHESS works by melting a PCM during the charging period and releasing this energy during discharging to heat the domestic hot water [2]. Figure 1 shows a schematic of a SDHW system.

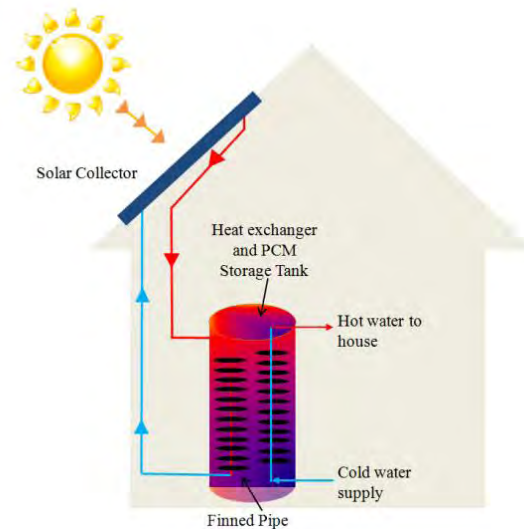


Figure 1. Schematic of a solar domestic hot water system with a LHESS using PCM.

In order to reduce the cost of designing a LHESS, numerical studies of different designs can be used, however modeling phase change heat transfer requires taking into account the total energy balance through the PCM, especially at the phase change front. It must also account for the proper physical behavior of both the solid and liquid phase, and compute the ever changing position of the phase change interface, which are both an input and an output of the problem. In a

typical numerical study, some simplifications are usually necessary.

Also, due to the low thermal conductivity of PCMs, it is necessary to implement additions in order to increase heat transfer and system efficiency; such additions can take the form of fins added to the system, insertion of highly conductive particles to the PCM, etc [3].

Past numerical studies using COMSOL Multiphysics have found the optimized spacing for horizontal fins for a cylindrical LHESS [4] and the total amount of energy that can be stored in both latent and sensible form inside a cylindrical LHESS as a function of the number of fins added [5]. However these models assumed conductive heat transfer through the PCM, neglecting the role of natural convection heat transfer in the liquid PCM. This assumption, being mostly valid for small PCM cavities, it will result in an under prediction of the heat transfer rate in most systems. For this reason, a model is needed in which convective heat transfer is accounted for in the PCM liquid phase, conduction still dominating in the PCM solid phase.

This paper presents the results obtained from a numerical model built to simulate melting of a PCM where both conduction and convection heat transfer are accounted for. Numerical results for convection dominated melting in a PCM, performed by five groups of researchers and presented in a paper by Bertrand et. al. [6], are used to validate this COMSOL Multiphysics model. Through the study of this model, the effects of the following parameters on PCM melting interfaces have been looked at: fluid viscosity, thermal conductivity and the addition of fins.

2. Geometry and Material

The geometry used to validate this model is a 0.1 m by 0.1 m square enclosure containing octadecane as the PCM as presented in Oliver Bertrand et. al [6]. Initially, the entire PCM is solid at its melting temperature $T_o = T_m = 303$ K. At $t = 0$, the left wall is heated to a temperature $T_w = 313$ K, while the right wall is kept at the initial temperature T_m . The top and bottom walls are insulated. Figure 2 shows this geometry and the boundary conditions.

A user defined material was selected in COMSOL and the PCM properties were input. The following thermophysical properties of the PCM were used in accordance with Bertrand et al. [6].

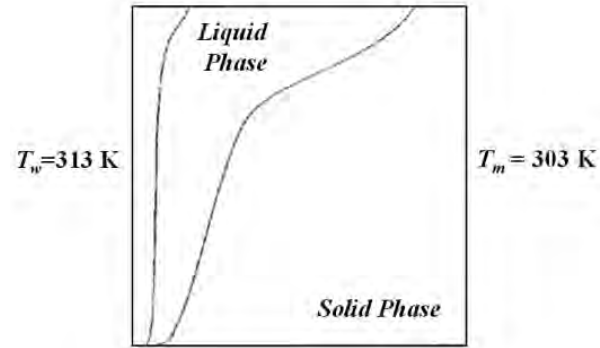


Figure 2. Problem geometry and boundary conditions [6].

Table 1. Thermophysical properties of octadecane use for the study [6].

Property	Value
Density	800 kg/m ³
Specific Heat	1,250 J/kgK
Latent Heat of Fusion	125,000 J/kg
Melting Temperature	303 K
Dynamic Viscosity	0.008 Pa·s
Thermal Conductivity	0.2 W/mK

3. Use of COMSOL Multiphysics

A 2D numerical study was performed in COMSOL Multiphysics (4.0a and 4.1) to simulate melting of a PCM including both conduction and convection heat transfer. The heat transfer in fluids and laminar flow physics interfaces were used. In order to model a change of phase in the material, several material parameters were adjusted as follows:

- I. To account for the latent heat absorbed during melting, a modified specific heat, C_p , was used, as described by Ogoh and Groulx [5] and seen in Eq. (1). A melting temperature range, ΔT_m , is used over which an adjusted specific heat acts. Over this melting temperature range, the modified specific heat accounts for both the latent heat of fusion and the sensible energy required to increase the temperature of the material. The modified specific heat and latent heat of fusion are shown for a 1 K melting range in Fig. 3.

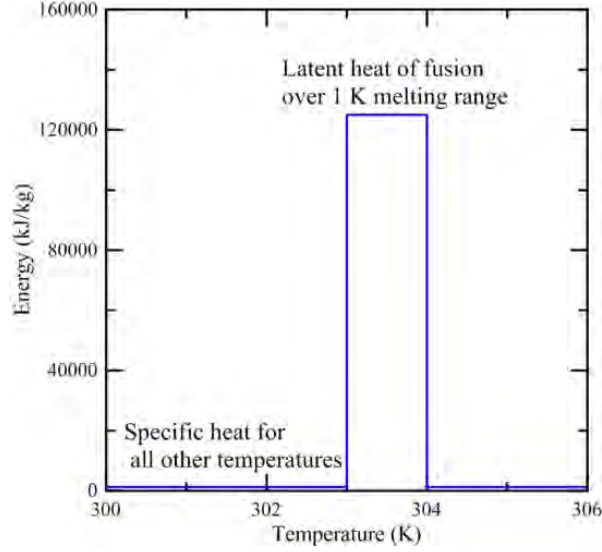


Figure 3. Modified specific heat.

$$c_p = \begin{cases} 1,250 \text{ J/kg} & \text{for } T < 303\text{K} \\ C_{pm} \text{ J/kg} & \text{for } 303 < T < 303\text{K} + \Delta T_m \\ 1,250 \text{ J/kg} & \text{for } T > 303\text{K} + \Delta T_m \end{cases} \quad (1)$$

The modified specific heat, C_{pm} , is calculated using the melting temperature range ΔT_m and the latent heat of fusion for the material L_f :

$$C_{pm} = \frac{L_f}{\Delta T_m} = \frac{125,000}{\Delta T_m} \quad (2)$$

This approximation is necessary since melting at an exact temperature cannot be modeled numerically. This also means the melting temperature range is selected by the user and can be varied.

- II. The dynamic viscosity, ν , 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 .

$$\nu = \begin{cases} 10^8 \text{ Pa}\cdot\text{s} & \text{for } T < 303\text{K} \\ 0.008 \text{ Pa}\cdot\text{s} & \text{for } T > 303\text{K} + \Delta T_m \end{cases} \quad (3)$$

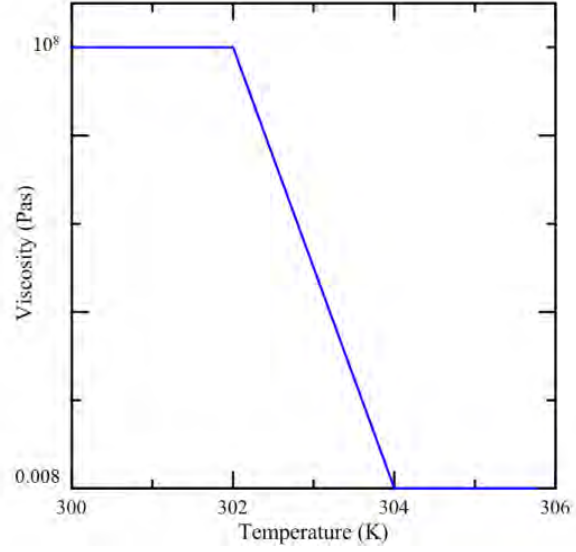


Figure 4. Modified dynamic viscosity.

A volume force was used to simulate the effects of density and gravity on the movement of the low viscosity fluid, and was calculated by:

$$F = g\rho\alpha(T - T_o) \quad (4)$$

Constant thermal conductivity and density values were used.

3.1 Model Mesh

2D quadrilateral elements were used to discretize the model. A mesh convergence study was done and as a result 4096 elements were selected giving an average element size of $2.44 \times 10^{-6} \text{ m}^2$. This element size provided convergence at a relatively low run time. Simulations took on average 7 hours on an Intel dual core processor.

4. Model Validation

Figure 5 presents the results after 5,000 s of simulated melting when using a temperature melting range of $\Delta T_m = 1 \text{ K}$. The result from the COMSOL convection model was as expected qualitatively: the melted PCM rises to the top of the enclosure as it gets heated, moves across the insulated top wall where it does not lose any heat, and then cools when it reaches the solid PCM. This cooler PCM falls and a recirculation pattern begins. This pattern is represented by the velocity arrows, and the melting interface is represented by the light dashed line in the COMSOL plot.

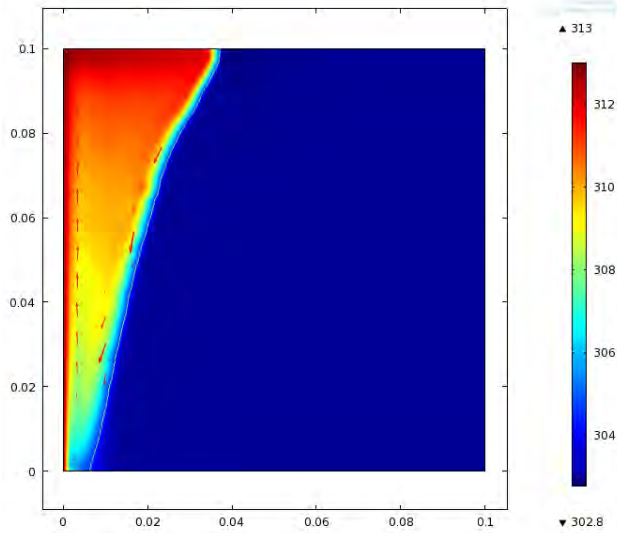


Figure 5. Melting interface and velocity profile at 5,000s for $\Delta T_m = 1$ K .

After 5,000 s from the onset of melting, 21% of the octadecane was melted. This melted fraction, MF , was calculated by taking a surface integral of the 2D system for every element having a temperature above $T_m + \Delta T_m/2$ and dividing by the total area of all elements:

$$MF = \frac{\iint_{Area\ with\ (T > T_m + \Delta T_m/2)} dx dy}{A_{tot}} \quad (5)$$

The position of the obtained melting interface was compared to two of the melting interface positions presented in Bertrand et al. [6]; those of Lacroix and Binet-Lacroix. Figure 6 compares those melting interface positions on a graph using a set of normalized axis.

The COMSOL model shows less melting than the reported results; however the melting interface shape is similar to that of Lacroix. This difference in position of the melting interface could be explained by the numerical definition of viscosity: from Fig. 4, a temperature close to 304 K must be reached before the PCM starts acting as a liquid, even if the mushy region is defined to be between 303 and 304 K. This delays the onset of natural convection close to the melting interface, resulting in less melting over time. Future simulations will look at the impact of the numerical definition of the viscosity on the overall melting of the PCM.

In order to validate a numerical model the results should also be compared to experimental data, which was unavailable for this study.

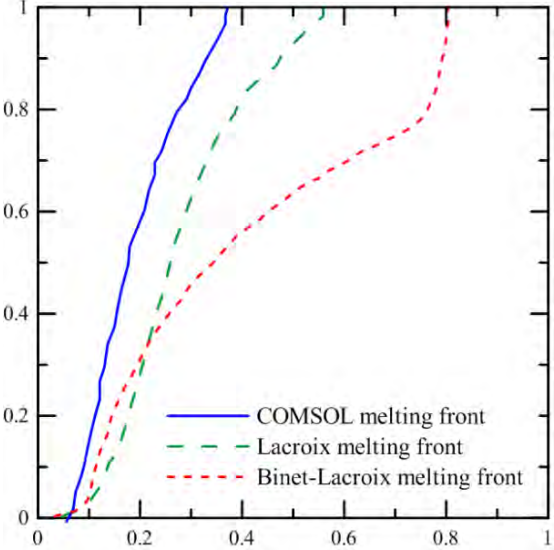


Figure 6. Melting interfaces compared with normalized axis at 5,000 s.

The effect of the melting temperature range on the melting interface position was studied for 0.01 K, 0.1 K, 0.25 K, 0.5 K, 1 K and 3 K melting temperature ranges. The results are presented in Fig. 7. Again, the same two interface positions from Bertrand et al. [6] are presented for reference.

The melting interfaces for the 0.1 and 0.5 K melting temperature ranges best fit the reported results from Bertrand et al. [6].

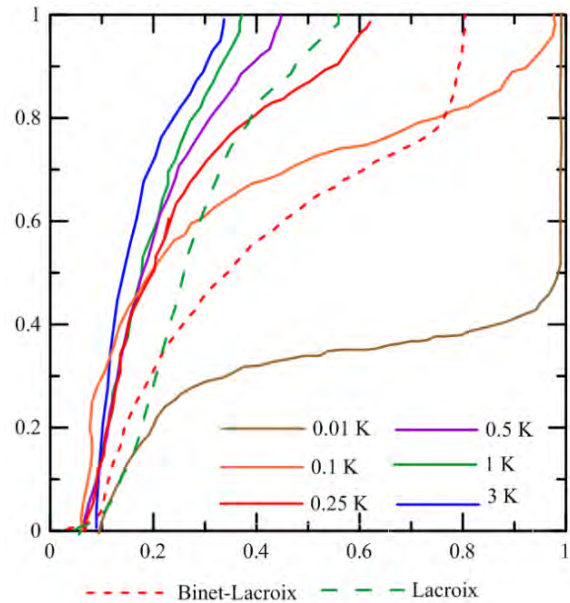
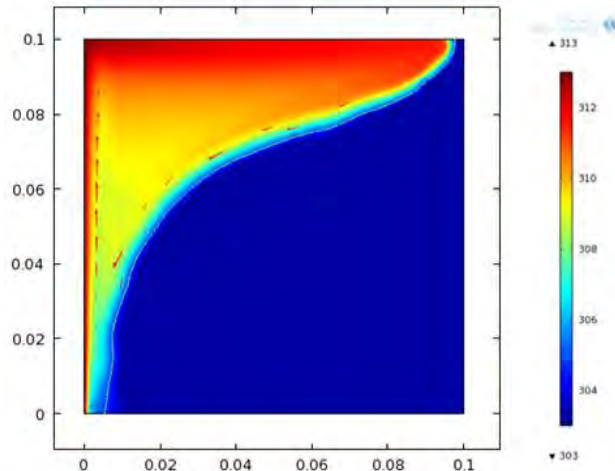
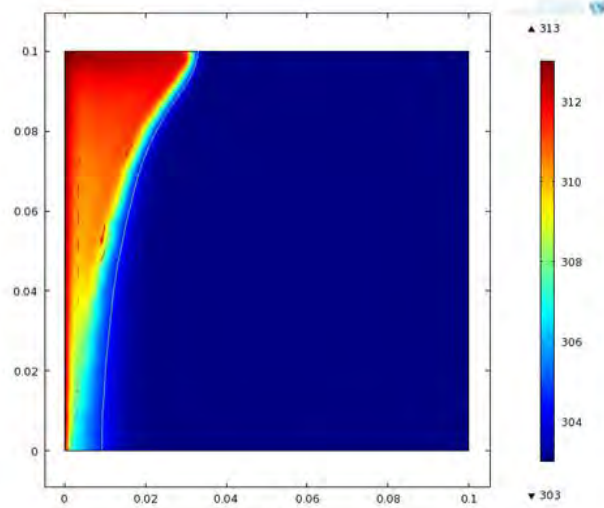


Figure 7. Melting interface position for varying ΔT_m after 5,000 s.



(a)



(b)

Figure 8. Melting interface and velocity profile after 5,000 s for a) $\Delta T_m = 0.1$ K, and b) $\Delta T_m = 3$ K.

Figure 8a) shows the melting interface position and temperature in the system when the melting temperature range is $\Delta T_m = 0.1$ K. The viscosity function being modified accordingly, the PCM starts behaving as a liquid at a temperature close to 303.1 K. As a result, natural convection starts to act faster near the melting interface, increasing the overall amount of melting in the system.

Figure 8b) shows exactly the opposite case, in which a $\Delta T_m = 3$ K results in less melting after 5,000 s mainly because natural convection is greatly delayed by the smaller amount of PCM acting as liquid.

This is an important trend to notice, as it shows the importance of natural convection, and the impact of the viscosity function definition, on

the melting phase of a PCM used for latent heat storage.

5. Parametric Analysis

The effects of material selection and fin additions were studied using the COMSOL convection model. For all of the following studies, $\Delta T_m = 1$ K was used.

5.1 Thermal Conductivity

Figure 9 shows the result obtained for a melting temperature range of 1 K and a thermal conductivity of 2 W/m·K, 10 times larger than that of octadecane. The larger thermal conductivity increased the amount of PCM that melted, as expected. A large natural convection cell is observed after 5,000 s of melting; nevertheless, the PCM remains solid close to the top of the right wall and the bottom right portion of the enclosure since the right wall is maintained at the melting temperature, 303 K.

With a thermal conductivity of 20 W/m·K, 100 times larger than octadecane, almost all the PCM was melted before the first 500 s, after which the liquid PCM continued to circulate in the enclosure.

This shows that convection still plays a role even when the thermal conductivity of the PCM is high. Unfortunately, most PCMs have very low thermal conductivities.

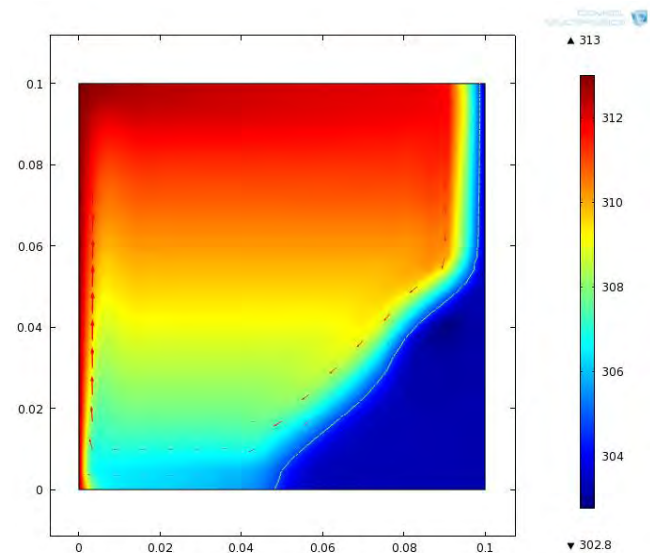


Figure 9. Melting interface and velocity for a thermal conductivity of 2 W/m·K after 5,000 s.

5.2 Dynamic Viscosity

The effect of PCM dynamic viscosity on the melting front was also studied, and it was found that for lower viscosities there is more melting along the top of the container due a decrease in the liquid PCM flow resistance that leads to increased natural convection, as seen in Figure 10. A higher viscosity makes the liquid PCM behaves less like a liquid, a somewhat more like a solid, resulting in a fairly vertical melting interface position akin to what is observed when natural convection is not modeled.

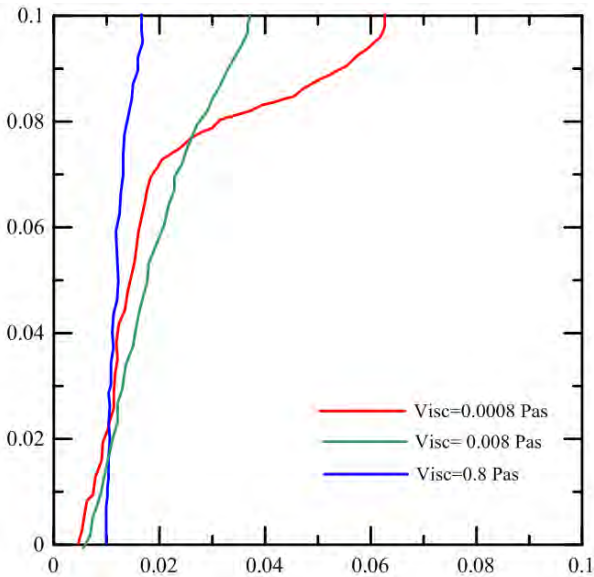


Figure 10. Melting interface position for varying viscosity values after 5,000 s.

5.3 Fin additions

A fin was added to the PCM enclosure to study the effects of the addition of a material with a higher thermal conductivity than the PCM used. Aluminum was used, which has a conductivity of 160 W/m·K. The resulting melting interface is presented in Fig. 11.

The fin increased the heat transfer through the PCM, as expected. More melting was seen in both the top and bottom compartments. In the bottom compartment, natural convection was increased by the increased heat transfer from the fin to the layer of liquid moving under it. Thermal plumes can also be observed on the top of the fin, increasing the amount of energy transfer to the top compartment.

At 5,000 s, 30% of the PCM was melted, which is a 9% increase over the case with no fin, which had a melted fraction of 21% at 5,000 s.

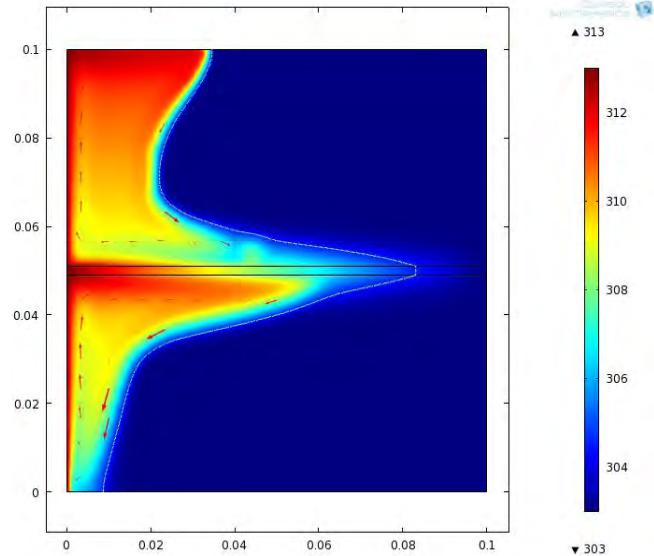


Figure 11. PCM melting with Aluminum fin.

6. Conclusions

Natural convection in the liquid phase of a PCM (octadecane) during melting was modeled using COMSOL Multiphysics. The natural convection model showed slightly less melting than the numerical studies presented by Bertrand et al. [6], however the same melting front shape was observed.

The impact of the melting temperature range used in the simulation was demonstrated. As well, the effect of the numerical definition of viscosity on the onset and strength of natural convection, and the resulting melting interface position, was discussed. Future studies will aim to quantify this effect and provide a combination of melting temperature range and numerical viscosity definition that provide the most accurate results.

The effects of viscosity and thermal conductivity of the PCM were studied as well, and changes in those material properties resulted in variations in the amount of PCM melted, as well as the shape of the melting front. However, the material properties of the PCM used in LHESS are fixed, therefore the addition of fins will be a good way to increase melting and encourage natural convection in the PCM.

7. References

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8. Acknowledgements

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