

An Analysis of Heat Conduction with Phase Change during the Solidification of Copper

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Abstract: The goal of this study was to determine the possibility of using the finite element in COMSOL Multiphysics program to obtain a high accuracy solution to a moving boundary problem, specifically, the solidification of copper. A one-dimensional geometry in Cartesian coordinates was used to investigate the solidification of initially liquid copper from a chilled wall maintained at fixed temperature. The other boundary was assumed adiabatic. Analytical and finite difference methods were also employed to solve the problem and to create a basis for comparison. Accurate solutions can be obtained using COMSOL Multiphysics but only after carefully tuning the solution parameters, particularly the time step. A limited number of computer experiments were then carried out to investigate the solidification problem in two dimensions for which no analytical solutions exist.

Keywords: Phase Change, Solidification, Effective Heat Capacity

1. Introduction

Phase change phenomena in materials are often encountered during the course of their manufacture, particularly metals. In the case of metals, at least two phase changes occur during the creation of the base material. Initially, the material must be smelted from the ore that has been removed from the earth in order to obtain a liquid metal. Subsequently, a second phase change is required to obtain a solid ingot from the molten metal previously obtained. It is frequently required that additional phase changes be used in the creation of finished products, as is true in the formation of all types of castings. Problems involving phase changes are also known as moving boundary problems since a key feature is the presence of a boundary separating the phases involved that changes position with time. At the moving boundary, the phases coexist and extraction of latent heat of phase

change is required for the boundary to move. From a practical standpoint, it is important to be able to accurately predict the instantaneous location of the moving boundary. Since the position of the moving boundary depends on the temperature field and this field in turn depends on the location of the boundary, solidification problems are non-linear and few analytical solutions exist. Moreover, the ones that exist are of limited practical use. Therefore, it is useful to have available numerical approximation methods capable of producing reliable solutions to solidification problems.

The particular problem being analyzed in this project is that of the time dependent heat conduction with solidification in copper. The conditions assumed for the analysis are that initially all the copper has been uniformly heated to a temperature above its melting point of 1356 K. The liquid copper is assumed to be contained between insulated horizontal walls and to be semi-infinite in the x-direction. Thermal energy is extracted from the system by imposing a temperature below the melting point at $x=0$. A schematic representation of the system is shown in Figure 1.



Figure 1: Depiction of Problem Definition

Two commonly used methods for the numerical solution of solidification problems are the effective heat capacity method and the enthalpy method. In both cases, the goal is to accurately represent the release of latent heat at the moving boundary. For instance, the enthalpy method has been used in phase change systems to determine the thermal performance of latent heat storage [1]. This same principle can be

utilized in the analysis of the solidification of copper. The ability for the enthalpy method to properly account for the latent heat lost during the solidification process makes it well suited to this scenario. Also, the effective heat capacity method has been proven capable of producing accurate solutions in studies of phase change phenomena. Since it is easy to account for temperature dependent thermal properties in COMSOL Multiphysics, the effective heat capacity method was used in this study.

2. Theory

The effective heat capacity method is based on the use of an apparent heat capacity over the melting range, directly proportional to the latent heat of phase change. Therefore, three temperature ranges of thermal capacitance within the system are obtained: above melting, during melting/solidification and below solidification. Although pure elements such as copper possess a unique melting point, an artificial melting range is required when using the effective heat capacity method. This range will have an effective heat capacity that is governed by (1) where, H_f is the latent heat of fusion and ΔT_f is the relatively small range of temperatures it is assumed that melting occurs over [1].

$$C_{p\text{ eff}} = \frac{H_f}{\Delta T_f} \quad (1)$$

The range of temperature is required to be chosen as small as possible in the case of pure metals in order to accurately represent the situation. However, the smaller the range the larger the jump in the value of the heat capacity and the larger the numerical difficulties encountered. The heat capacities for the single phase regions are simply defined by using the average of known values for the heat capacity of the solid and liquid phases, which are readily available.

The heat equation (2) is a parabolic partial differential equation which describes the distribution of temperature within a system as a function of time.

$$\frac{\partial v}{\partial t} = \kappa \cdot \nabla^2 \cdot v \quad (2)$$

In phase change systems, two such equations are required, one for the solid phase and one for the liquid phase. The heat equation is such that the system will have a maximum temperature within itself that is either defined as occurring at the initial time or occurring at one of the boundary locations. This property of the heat equation is important due to the fact that heat cannot be generated within the system without some kind of external heat source being added [2].

In order to obtain an exact analytical solution to a moving boundary problem that can be used to describe the problem being analyzed, it is required to write the heat equation for each phase and the following conditions at the solid – liquid interface, called Stefan conditions:

$$v_1 = v_2 = T_I, \text{ when } x = X(t) \quad (3)$$

$$K_1 \cdot \frac{\partial v_1}{\partial x} - K_2 \cdot \frac{\partial v_2}{\partial x} = H_f \cdot \rho \cdot \frac{d}{dt} \quad (4)$$

These conditions determine where the boundary separating liquid and solid material lies and account for the latent heat of phase change. Thus, for the system sketched in Fig. 1, this means that for $x > X$ the material is liquid at temperature $v_2(x,t)$ and for $x < X$ the material is solid of temperature $v_1(x,t)$. The Stefan conditions take into consideration the coexistence of the phases at the interface as well as the latent heat that must be removed or added in order for the phase change to occur and for the interface to move [3].

One specific solution that is particularly helpful in defining the temperature distribution found for the one dimensional situation to be analyzed here is the Neumann solution [3]. In this exact solution it is assumed that the region being analyzed is semi-infinite (i.e. extends from $x > 0$). Moreover, the initial temperature is V and the surface $x = 0$ is maintained at T_w for all times $t > 0$. In this solution set of equations, the boundary conditions are redefined to be:

$$v_2 \rightarrow V, \text{ as } x \rightarrow \infty \quad (5)$$

$$v_1 = T_w, \text{ when } x = 0 \quad (6)$$

Solution of the heat equation for the two phases together with the Stefan conditions yields the following transcendental equation for the solidification constant λ .

$$\frac{e^{-\lambda^2}}{\operatorname{erf}(\lambda)} - \frac{K_2 \cdot \kappa_1^{1/2} \cdot (V - T_1) \cdot e^{-\kappa_1 x^2 / \kappa_2}}{K_1 \cdot \kappa_2^{1/2} \cdot (T_1 - T_w) \cdot \operatorname{erfc}(\lambda \cdot (\kappa_1 / \kappa_2)^{1/2})} = \frac{\lambda \cdot H_f \cdot \pi^{1/2}}{c_1 \cdot (T_1 - T_w)} \quad (7)$$

The position of the solid – liquid interface is simply given by:

$$X = 2 \cdot \lambda \cdot (\kappa_1 \cdot t)^{1/2} \quad (8)$$

It is possible to obtain a curve that defines the exact solution for the Newmann problem. This solution can then be compared against various outputs from finite element analysis programs, such as COMSOL Multiphysics.

In addition to obtaining an equation defining the location of the solid – liquid interface it is also possible to obtain expressions that define the temperatures of the solid and liquid phases with respect to position and time, i.e.

$$v_1 = T_w + \frac{T_1 - T_w}{\operatorname{erf}(\lambda)} \cdot \operatorname{erf}\left(\frac{x}{2 \cdot (\kappa_1 \cdot t)^{1/2}}\right) \quad (9)$$

$$v_2 = V - \frac{(V - T_1)}{\operatorname{erfc}(\lambda \cdot (\frac{\kappa_1}{\kappa_2})^{1/2})} \cdot \operatorname{erfc}\left(\frac{x}{2 \cdot (\kappa_2 \cdot t)^{1/2}}\right) \quad (10)$$

3. One – Dimensional Analysis

3.1 Method

Figure 2 shows the computed position of the moving boundary calculated using the Newmann solution given above together with the data in Table 1. The figure shows that the solid-liquid interface moves steadily away from the origin as the material cools and solidification takes place.

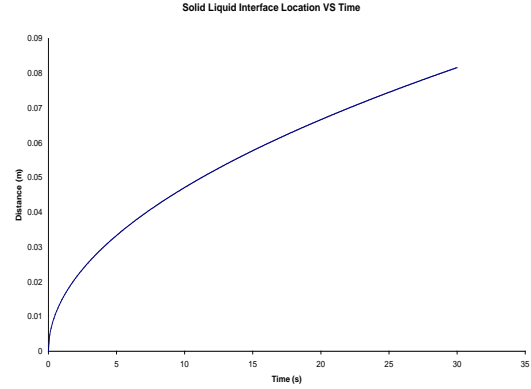


Figure 2: Solid – Liquid Interface location as function of time (Newmann solution).

As an example of a numerical approximation, a previously developed computer program implementing the enthalpy method with a simple explicit finite difference scheme was used to solve the same problem. The explicit method allows solving the finite difference equations using a time marching procedure to solve the finite difference equations, while the enthalpy formulation is used to handle the latent heat. The result of using the existing code for the solution of the problem considered in this study is compared with the analytical solution and shown in 3. The staircase appearance of the moving boundary location is a well know feature of solution obtained with the enthalpy method.

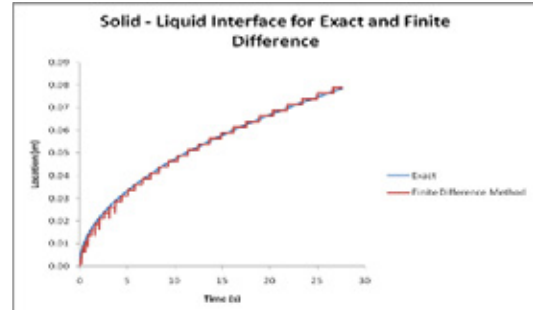


Figure 3: Comparison of finite difference and exact solutions.

The results show that the overall accuracy of prediction of the moving boundary location with the enthalpy method is approximately 3%.

The same system was then modeled using COMSOL Multiphysics. Initially, after entering

the input data, no modifications were made to the default solution parameters in COMSOL. More accurate solutions were obtained only after manual tuning of the time step used in the solution.

Table 1: Input Data

Property Name	Physical Property Symbol	Value
Thermal Conductivity	K_s, K_l	365, 174 W/m·K
Density	ρ	8920 kg/m ³
Specific Heat	C_{ps}, C_{peff}, C_{pl}	435, 10250, 494 J/kg·K
Melting Range	T_s, T_l	1350, 1360 K
Temperature Initial	V	1400 K
Temperature External	T_w	400 K

3.2 Results

As a test, an initial calculation was done using the COMSOL model but disregarding the variation of all the thermal properties with temperature and using a single average value in each case. Moreover, the latent heat was neglected altogether. The computed temperature profile is shown in Figure 4.

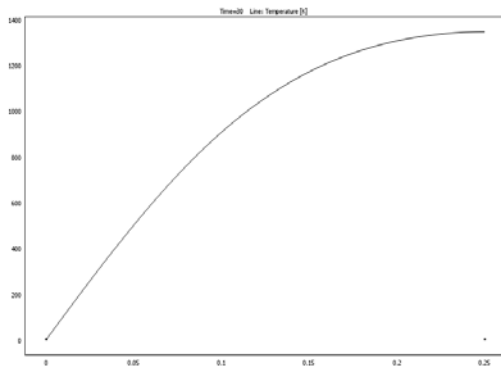


Figure 4: COMSOL plot of temperature vs. distance at t=30 s (no latent heat).

The resulting temperature distribution is smooth and since the latent heat was neglected, there is no evidence of moving boundary. This is not the case when the latent heat is taken into account, like in the analytical solution, where a distinct “knee” appears on the curve at the location of the solid-liquid interface. When the latent heat is incorporated into the model through the use of the effective heat capacity when the temperature is inside the melting range, as well as the appropriate values of thermal conductivity for the solid and liquid phases, it is possible to create an accurate and meaningful representation of the heat transfer through the material over time including the instantaneous location of the moving boundary. The result of this calculation is shown in Figure 5.

When the correct set of temperature dependent properties are used in the COMSOL model, three distinct regions are formed. As the thermal conductivity and heat capacity of liquid and solid copper are not equal and since removal of heat is required for the interface to advance, the temperature profile above the melting point has a certain slope, while below the melting point, the slope is different, as seen in Figure 5.

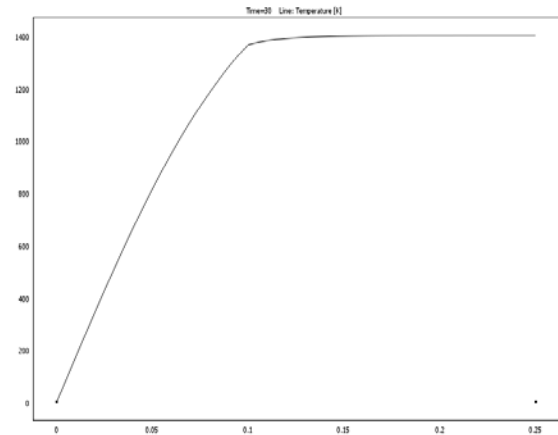


Figure 5: COMSOL plot of temperature vs. distance at t=30 s (with latent heat)

In creating these results no properties were altered from the previous case with the exception of including the appropriate thermal conductivity values and the effective heat capacity. By using the correct values of thermal conductivity and

heat capacity, the results were much improved over the initial test analysis.

A series of six improved solutions were created with identical material properties, and by only altering the time step used in the solution method. The time step for the solution is the way in which the COMSOL Multiphysics program chooses to divide a transient analysis. This parameter can be modified in order to obtain a solution that can more accurately describe a transient phenomenon. Table 2 below shows the six variations chosen for this analysis. It is important to note that while decreasing the time step for the solution can possibly improve the accuracy of the results, it also greatly increases the execution time and memory requirements for the analysis.

Table 2: Transient Analysis Time Step Options

Option	Time Step Name	Initial Step	Max Step
1	Free	-	-
2	Intermediate	-	-
3	Strict	-	-
4	Manual	.001	.01
5	Manual	.0001	.001
6	Manual	.00001	.0001

While this depiction of the temperature over the region being analyzed is a helpful indication that the incorporation of latent heat produced a more realistic solution, it is necessary to compare the solid – liquid interface location calculated from the exact solution against the one computed with COMSOL Multiphysics. In order to do this, values for the solid – liquid interface were found at intervals over the transient solution up to 30 seconds. The resulting solutions for the six cases in Table 2 are shown in Figure 6. This plot was created by exporting the raw solution data from COMSOL Multiphysics for each time step option into Excel and overlaying the results.

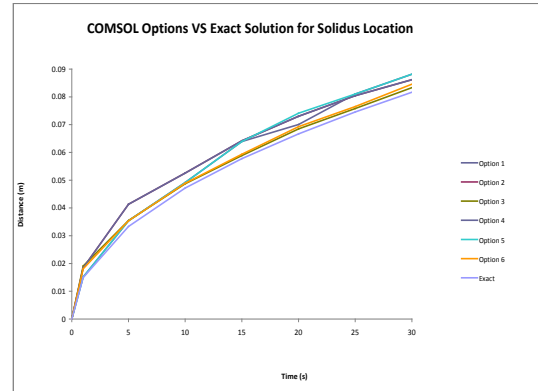


Figure 6: Comparison of COMSOL solutions to exact solution for solid – liquid interface location

In addition to the visual comparison in Figure 6 above, an analytical comparison of the percent difference between the individual points from the COMSOL Multiphysics solutions and the corresponding exact solution points was determined using equation 11.

$$\% \text{ Difference} = \frac{x_{COMSOL} - x_{Exact}}{\left(\frac{x_{COMSOL} + x_{Exact}}{2}\right)} \times 100 \quad (11)$$

These individual percent differences were then averaged to obtain the average percent difference for each of the options. The results are shown in Table 3 below.

Table 3: Average percent difference in solid – liquid interface location compared to exact solution

Option	Average Percent Difference
1	6.07 %
2	12.28 %
3	6.03 %
4	12.28 %
5	6.87 %
6	5.92 %

Similar to what was shown in Figure 6, the overall percent difference between the exact

solution and the COMSOL solution for Option 6 gives the highest accuracy solution for solid – liquid interface location. The accuracy of the solution that defines the solid – liquid interface location is comparable to those seen in the finite difference method but does not exhibit the staircase appearance associated with the enthalpy method.

The one – dimensional solution that is obtained by incorporating the effective heat capacity method to the COMSOL Multiphysics program is such that the solution is of a significantly higher accuracy than what was initially obtained by neglecting the effect of the latent heat with only minor changes to the standard COMSOL program by introducing two temperature dependent functions. The resulting COMSOL Multiphysics solution is of accuracy comparable to the one obtained using the explicit, finite difference enthalpy method, as shown in Figure 7 below.

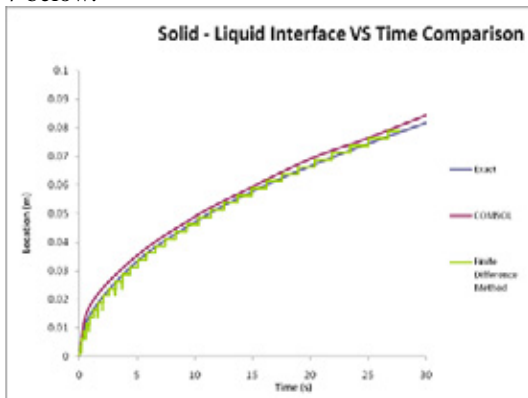


Figure 7: Comparison of FDM, COMSOL and Exact Solid – Liquid Interface Locations

In addition to the alteration of the defining material properties, the use of an appropriate time step interval is required to complete the transient analysis within COMSOL Multiphysics. It has been shown that the resulting solution from COMSOL Multiphysics program with a manual time step with an initial time step of .00001 seconds and a maximum time step of .0001 seconds was able to describe the location of the solidus to within 6% overall accuracy during the initial 30 seconds of the solidification process. It is important to note that the improvement in the interface location over time between the six solution methods cannot be determined to be

proportionately significant. Additional work should be completed in the form of testing of other systems and actual temperature results compared to COMSOL solutions in order to obtain more significant results proving the necessity of utilizing a time step analysis such as Option 6, which takes a large period of time to complete, even in such a simplified system.

4. Two – Dimensional Analysis

While an exact solution can be obtained for the one – dimensional system identified, no such exact solution exists for any two – dimensional system. In order to obtain a data point to compare the COMSOL Multiphysics solution, it is required to choose a system that can be related back to the only exact solution that exists. For this reason the system shown in Figure 8 was selected. The sketch shows a two-dimensional region exposed to chilled walls at the lines $x=0$ and $y=0$ and insulated at the other two boundaries.

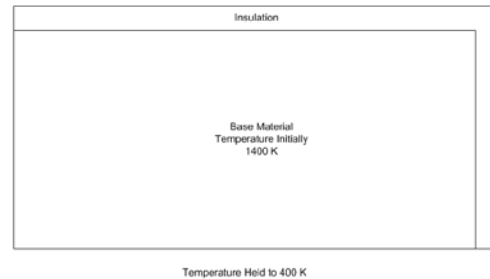


Figure 8: Depiction of 2D system being analyzed

Using this setting it is possible to create a correlation between the one - dimensional analysis that has been validated and the two - dimensional analysis. By creating the correlation back to the one - dimensional analysis it can be assumed that the parameters used are accurate for multiple scenarios and appropriate for most freezing analyses in a copper system. The goal of the two - dimensional analysis is to accurately describe the freezing within the system such that along the walls far from the corner, the obtained solution shall closely match the solution that was obtained in the one – dimensional system. While

the results from the one – dimensional analysis determined the need to use a small time step to obtain an accurate solution, two time step intervals were chosen to be used in the two – dimensional analysis, the strict time step and the manual .00001 initial and .0001 max time step. A COMSOL model representing the sketch shown in Figure 8 was created. Using the input data in Table 1 and the strict time step method produced the temperature field shown in Figure 9 below after 30 seconds of elapsed time.

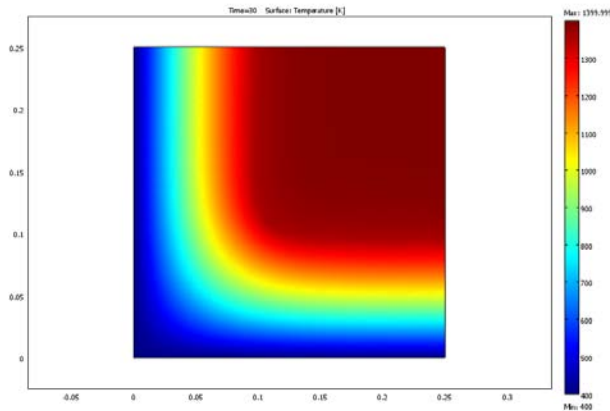


Figure 9: COMSOL computed temperature field for t=30 s.

This plot is in keeping with the expected results of heat conducting through the system into the surrounding cooler areas.

Using this output it was again required to compute the interface location within the system as a function of time for both the x and y directions and to compare these results to those of the exact solution and the optimized one – dimensional solution. This was done and the results are shown in Figure 10.

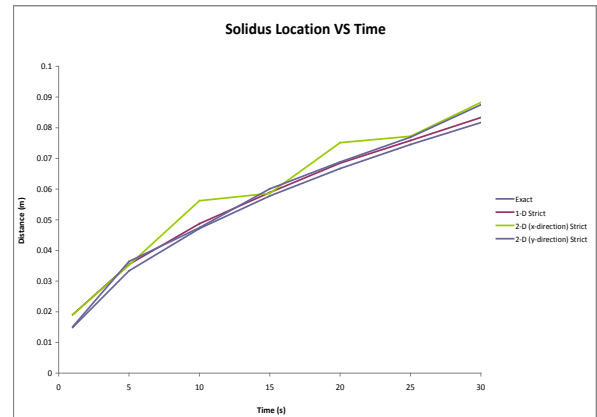


Figure 10: Solid – liquid interface location comparison (2D and 1D)

It can be seen from these results that the x-direction results of the two – dimensional analysis has significantly more error than that of the similar one – dimensional analysis and the two – dimensional analysis in the y-direction. The percent differences between the strict two – dimensional analysis and the exact solution are shown in Table 4.

Table 4: Percent Difference between 2-D Strict and Exact 1-D Solid – Liquid Interface Location

Direction	Percent Difference
x	10.30 %
y	4.00 %

In attempts to implement the manual time step solution for the two – dimensional analysis for a .0001 time step, the computational power required by the system to solve this problem was not available in the computers used to perform this analysis. Due to this fact no results were obtained for this solution set and all figures and calculations above were created using the less accurate strict time step interval.

7. Conclusions

The results of this study indicate that the use of the COMSOL Multiphysics to create accurate representations of the problem of heat conduction with phase change in a copper system

is promising. While the range of this study was not enough to definitively show the high accuracy results that are required in many real world applications, the results show the potential for a use of this concept in creating high accuracy models.

The study showed that by introducing two simple functions to define the thermal conductivity and most importantly the specific heat of copper, one was able to greatly increase the ability for COMSOL Multiphysics to predict the thermal behavior of copper as it solidifies. The introduction of these functions made possible to create a model where the latent heat of solidification was able to be accurately accounted.

With additional modification of parameters and the availability of high power computers, work can be continued to optimize this concept and create a fully developed high accuracy model of the solidification of copper within COMSOL Multiphysics. In addition to more computational work, the use of testing to create a series of sample sets where the actual inputs and outputs of the system are known would greatly increase the validity of this method.

It has been shown in this study that the concept of altering the COMSOL Multiphysics program moderately, can have a significant positive impact on the solution approximation that is created. It can be deduced that in further time it will be possible to create a heat transfer program that is able to properly define any phase change phenomenon within a system with the addition of a few new parameter inputs.

8. References

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