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

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COMSOL-09

Scope

- Use COMSOL to predict and visualize heat transfer including phase change
- Correlate known exact solutions for phase change to solutions created using COMSOL
- Work carried out to fulfill requirements for the Masters degree in Mechanical Engineering at Rensselaer-Hartford.

Background

- Phase changes occur in the production and manufacture of metals
- Phase change, or moving boundary, problems are non-linear and few analytical solutions exist

Governing Equations

Heat Equation (for Solid and Liquid Phases)

$$\delta H/\delta t = \mathrm{div}\ (k\ \mathrm{grad}\ T)$$

Thermal equilibrium at solid-liquid interface

$$v_1 = v_2 = T_1 \text{ when } x = X(t)$$

Stefan condition at the solid – liquid interface to define its location accounting for latent heat

$$K_1 \cdot \frac{\partial v_1}{\partial x} - K_2 \cdot \frac{\partial v_2}{\partial x} = H_f \cdot \rho \cdot \frac{d}{d}$$

Governing Equations

Newmann obtained an exact solution for the solidification of a semi-infinite liquid region starting at a chilled wall

$$v_2 \to V\text{, as x} \to \infty$$

$$v_1 = T_{\text{w}}\text{, when x} = 0$$

Incorporation of the Stefan condition yields an equation for the solidification constant λ

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

Governing Equations

The solidification constant is used to calculate the position of the solid – liquid interface, X, as a function of time

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

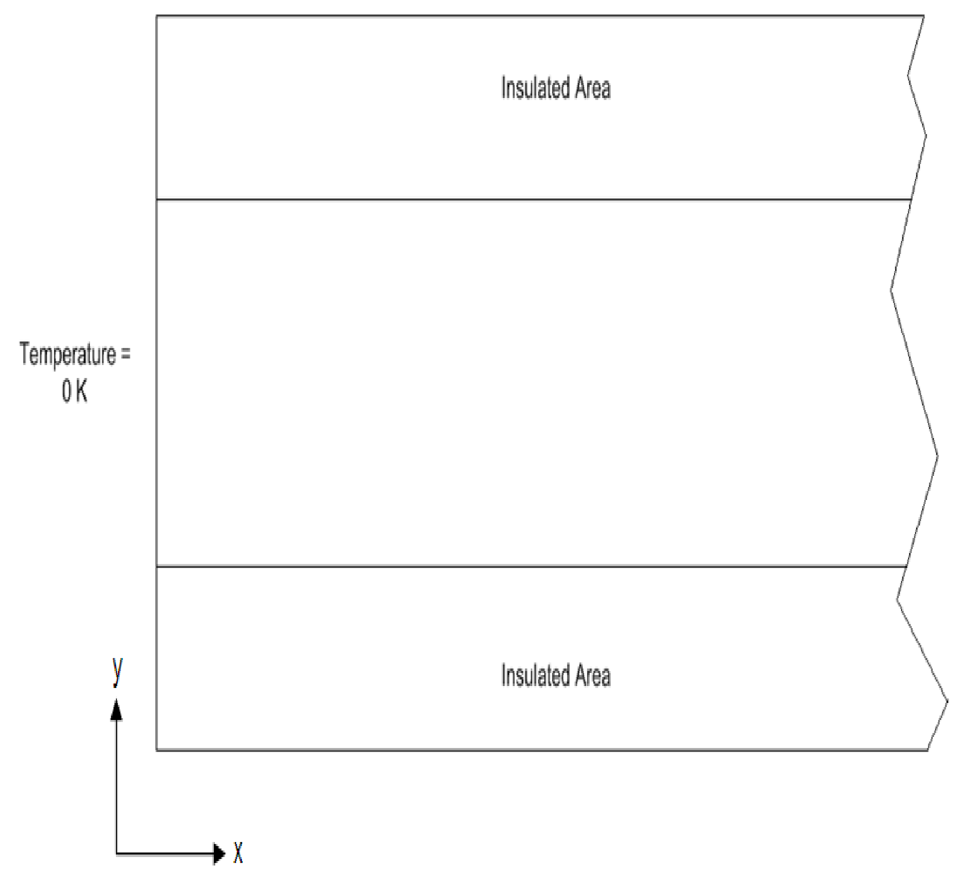
$$v_1 = T_w + \frac{T_1 - T_w}{erf(\lambda)} \cdot erf(\frac{x}{2 \cdot (\kappa_1 \cdot t^{1/2})})$$

In addition, it is also used to define the solid phase and liquid phase temperatures with respect to time and position

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

One – Dimensional Analysis Model Creation

- A one – dimensional model was created in COMSOL to model solidification of pure copper
  - Initial temperature = 1400 K
  - Temperature at Cold Wall = 400K
- Thermal conductivity and specific heat were created first as constants and then as temperature dependent variables



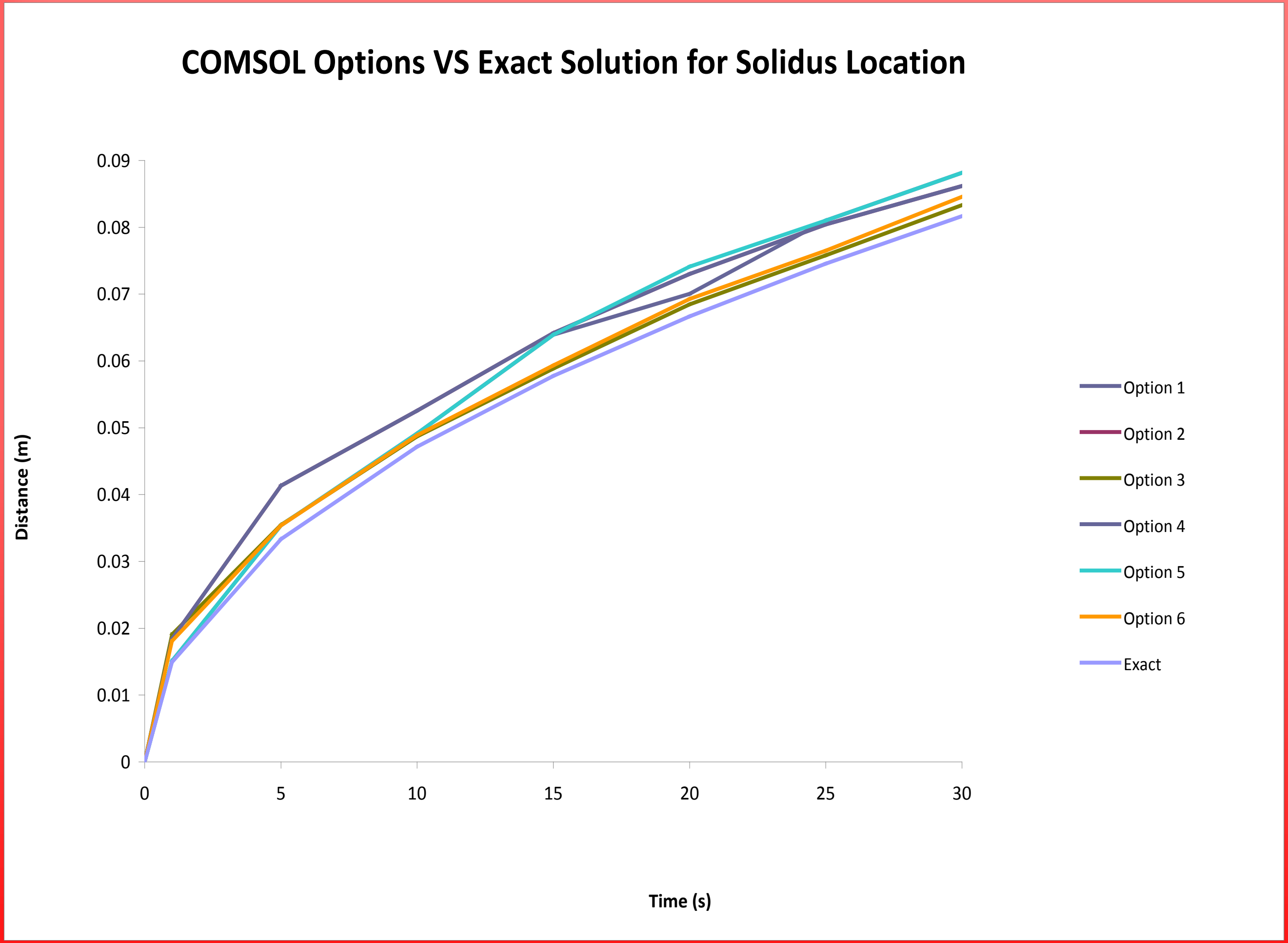
One – Dimensional Analysis Model Validation

- Results from COMSOL were compared to the analytical solution and with the results of a finite difference solution
- COMSOL results were obtained using a series of transient time step analysis options. Decreasing the time step increased the accuracy of the solution
- The percent difference from the analytical solution was determined using the following equation:

$$\%Difference = \frac{x_{COMSOL} - x_{Exact}}{(\frac{x_{COMSOL} + x_{Exact}}{2})} \times 100$$

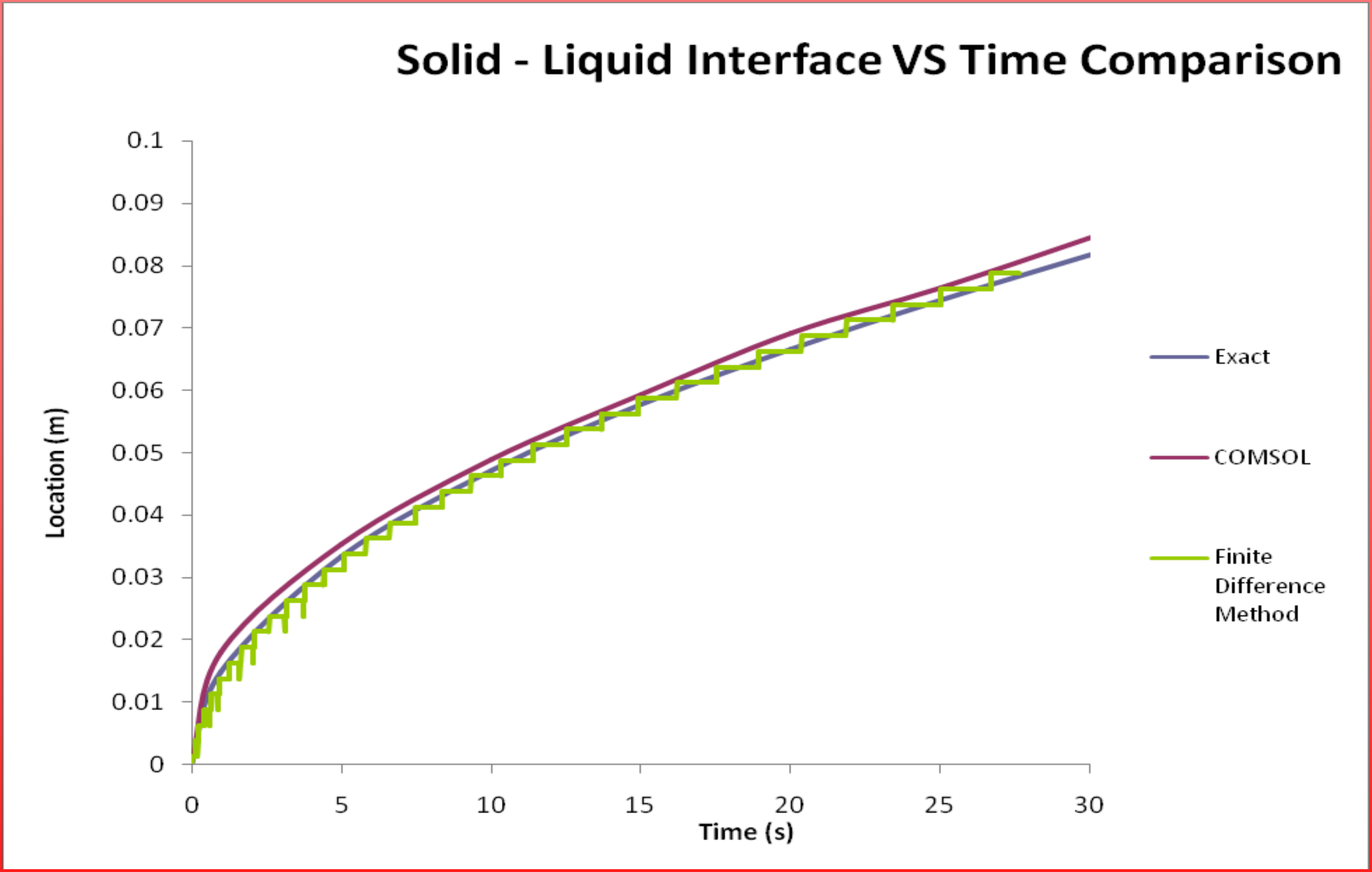
Option	Time Step Name	Initial Step	Max Step
1	Free	-	-
2	Intermediate	-	-
3	Strict	-	-
4	Manual	.001	.01
5	Manual	.0001	.001
6	Manual	.00001	.0001

Predicted S-L Interface Location COMSOL vs. Analytical



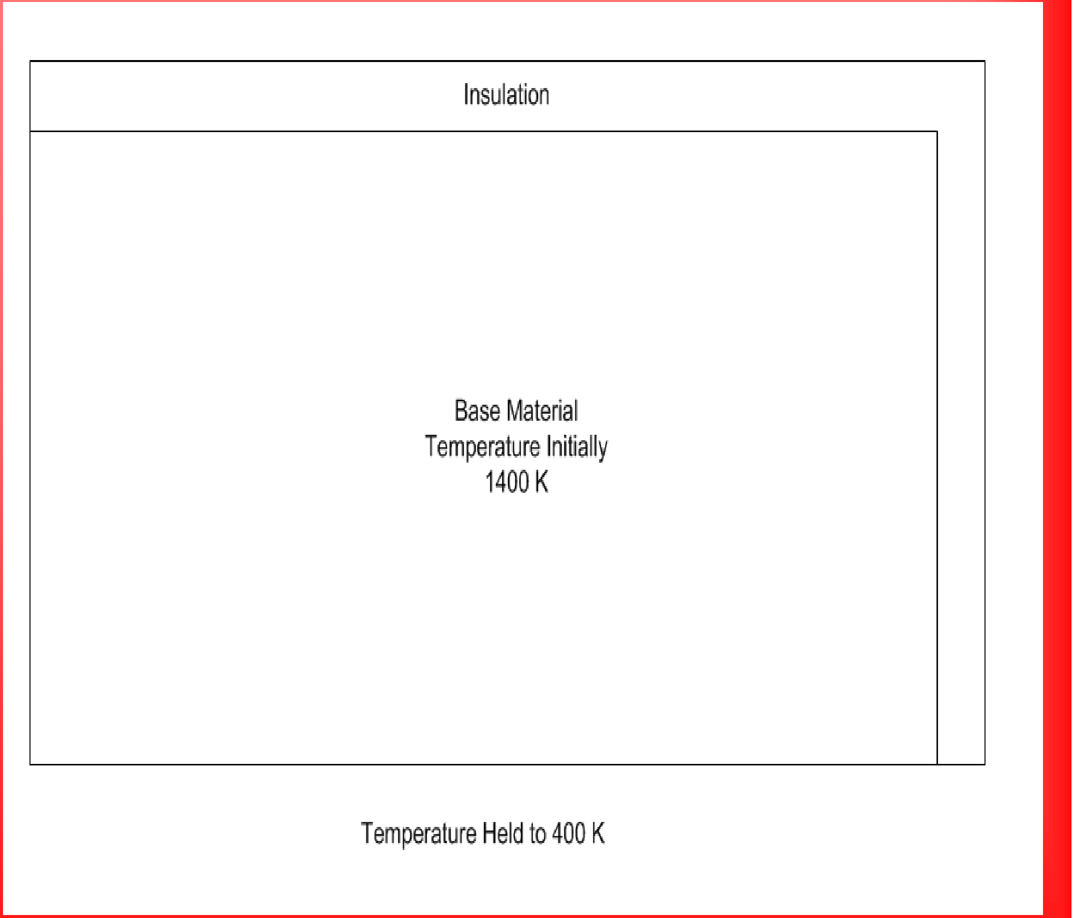
Option	Average Percent Difference
1	6.07 %
2	12.28 %
3	6.03 %
4	12.28 %
5	6.87 %
6	5.92 %

Predicted S-L Interface Location COMSOL, Analytical, FDM



Two – Dimensional Analysis Model Creation

- A two – dimensional model was also created in COMSOL
  - Initial temperature = 1400 K
  - Temperature at Cold Walls = 400 K
  - Two perpendicular sides assumed to be perfectly insulated
- The two – dimensional system should behave similarly to the previous one – dimensional case along the lines x = L and y = L

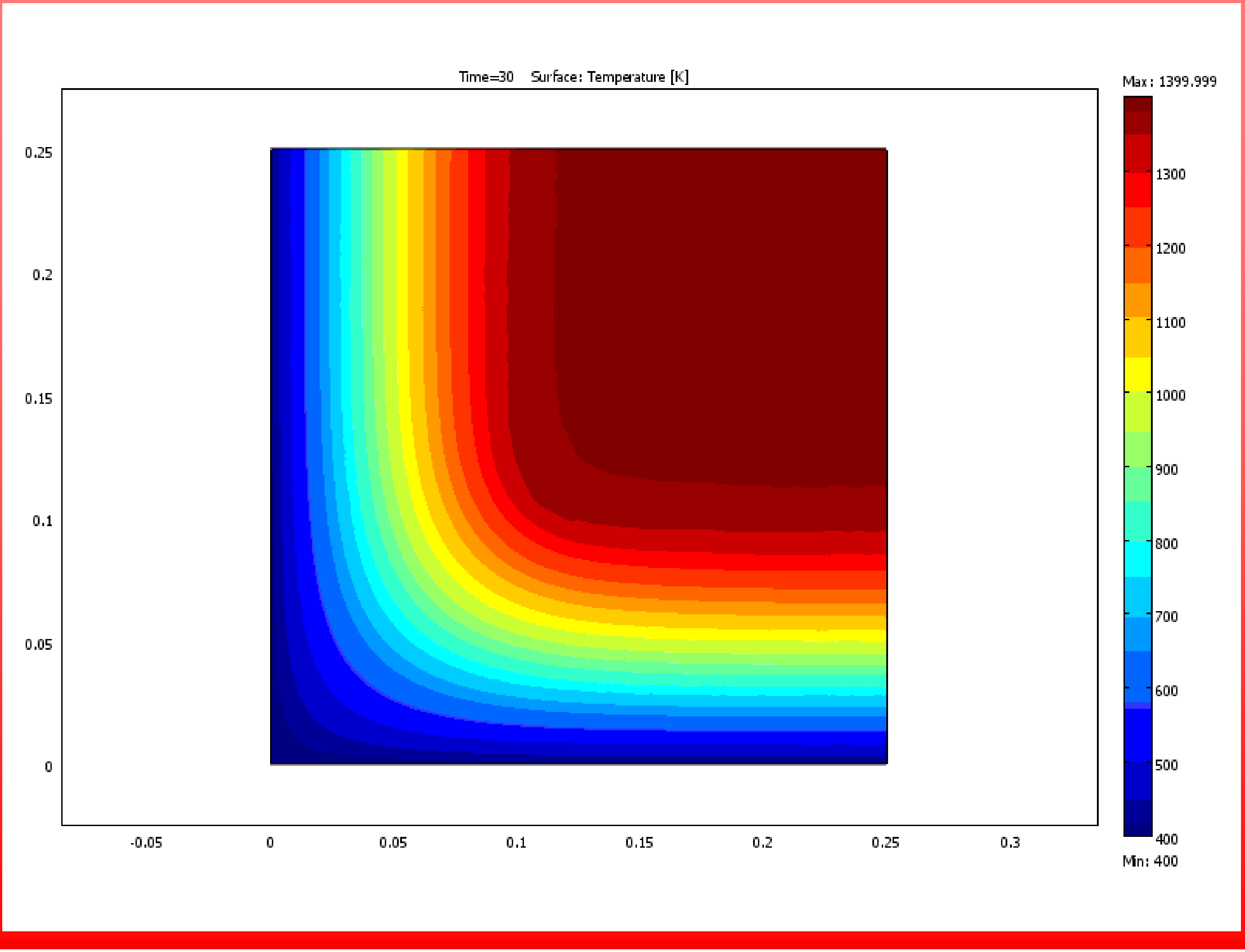


Two – Dimensional Analysis Model Validation

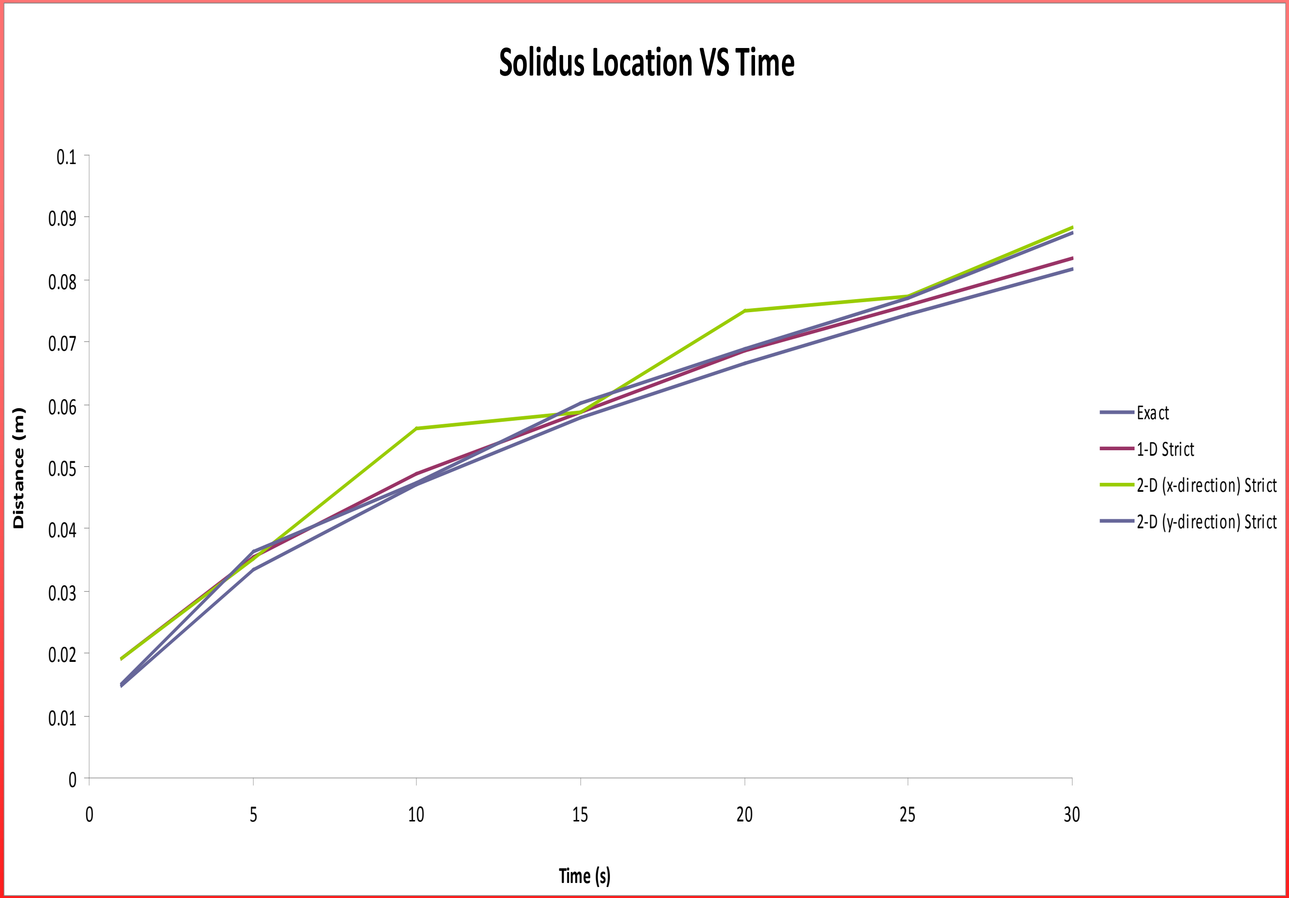
- COMSOL results were created using one of the best options obtained in the one – dimensional analysis; the strict time step
- Results from COMSOL two – dimensional analysis were compared to analytical solutions obtained for the previous, one – dimensional case in the x and y – directions
- The percent difference from the analytical solution was determined using the following equation:

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

Predicted Temperature Profile



Predicted S-L Interface Location COMSOL 2D Model



Direction	Percent Difference
x	10.30 %
y	4.00 %

Conclusions

- COMSOL shows promise as an easy to use tool for the creation of accurate representations of problems involving heat conduction with change of phase.

- The introduction of two simple functions defining thermal conductivity and specific heat as functions of temperature readily allows for the incorporation of latent heat effects in a COMSOL conduction heat transfer model and makes possible accurate predictions of the solid-liquid interface location in 1D systems.

- Additional work should be done to optimize this concept including correlating the results to actual test data, particularly for multi-dimensional systems.