Transient Heat Response of a 2-Phase System

Problem statement

In order to apply tighter control on a 6 in line (6IL) furnace a predictive model was built. The model currently does not take into account transient effects when calculating the melting rate. This is causes inaccuracies particularly when the input power changes drastically like when a start up or shut down is happening.

Solution Proposal

Create a heat conduction solver capable of modelling transient scenarios with phase changes.

Literature Review

For the transient component of the solver the implicit scheme will be used. This theme offers better stability over larger time steps (H.K Versteeg 2007). This scheme has an additional advantage exactly the same as the steady state scheme except that the specific enthalpy present in the cell is allowed to change with each iteration e.g. $\dot{h} \neq 0$.

General purpose Transient conduction model with 2 phases

Discretized Equation

Transient Conduction

Equation 1: Differential equation of transient heat conduction

$$\dot{h} = \frac{\partial^2}{\partial x^2}\left(\frac{k}{\rho}T\right) + \frac{\partial^2}{\partial y^2}\left(\frac{k}{\rho}T\right) + \frac{\partial^2}{\partial z^2}\left(\frac{k}{\rho}T\right) + \dot{q}$$

Discretizing the specific enthalpy rate term over time gives:

Equation 2: Discretized specific enthalpy rate

$$\dot{h} = \frac{h(T_t) - h(T_{t-\Delta t})}{\Delta t}$$

Where:

$T_t = The\ temperature\ at\ the\ center\ of\ the\ current\ cell\ at\ the\ current\ timestep\ [K]$

$T_{t-\Delta t} = The\ temperature\ at\ the\ center\ of\ the\ current\ cell\ at\ the\ previous\ timestep\ [K]$

$\Delta t = The\ size\ of\ the\ time\ step\ [s]$

$h(T) = The\ specific\ entalpy\ of\ the\ current\ cell\ at\ the\ given\ temperature\ \left[\frac{J}{kg}\right]$

The power generated by the cell will be given as a parameter of the model. From this the specific power generated is calculated as such:

Equation 3: Specific power generation definition

$$\dot{q} = \frac{\dot{Q}}{m}$$

Where:

$\dot{Q} = The\ power\ generated\ by\ the\ current\ cell\ [W]$

$m = The\ mass\ of\ the\ current\ cell\ [kg]$

Discretizing the conduction terms over their spacial dimensions gives:

Equation 4: Discretization of the x conduction term

$$\frac{\partial^2}{\partial x^2}\left(\frac{k}{\rho}T\right) = \frac{\frac{\partial}{\partial x}\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{West}\right]}{\Delta x_{Cell}} = \frac{\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta x_{East} \times \Delta x_{Cell}} - \frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{West}\right]}{\Delta x_{West} \times \Delta x_{Cell}}$$

Equation 5: Discretization of the y conduction term

$$\frac{\partial^2}{\partial y^2}\left(\frac{k}{\rho}T\right) = \frac{\frac{\partial}{\partial y}\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{South}\right]}{\Delta y_{Cell}} = \frac{\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta y_{North} \times \Delta y_{Cell}} - \frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{South}\right]}{\Delta y_{South} \times \Delta y_{Cell}}$$

Equation 6: Discretization of the z conduction term

$$\frac{\partial^2}{\partial z^2}\left(\frac{k}{\rho}T\right) = \frac{\frac{\partial}{\partial z}\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Bottom}\right]}{\Delta z_{Cell}} = \frac{\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta z_{Top} \times \Delta z_{Cell}} - \frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{Bottom}\right]}{\Delta z_{Bottom} \times \Delta z_{Cell}}$$

Where:

$k = Conduction\ coeficient\ \left[\frac{W}{m \times K}\right]$

$\rho = Density\ \left[\frac{kg}{m^3}\right]$

$T = Temperature\ [K]$

$\left(\frac{k}{\rho}T\right)_{Subscript} = The\ conduction\ potential\ of\ the\ cell\ indicated\ by\ the\ subscript\ \left[\frac{W}{kg}m^2\right]$

$\Delta x_{Cell} = Cell\ width\ [m]$

$\Delta y_{Cell} = Cell\ length\ [m]$

$\Delta z_{Cell} = Cell\ height\ [m]$

$\Delta x_{East} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ eastern\ neighbour\ [m]$

$\Delta x_{West} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ western\ neighbour\ [m]$

$\Delta y_{North} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ northen\ neighbour\ [m]$

$\Delta y_{South} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ southern\ neighbour\ [m]$

$\Delta z_{Top} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ top\ neighbour\ [m]$

$\Delta z_{Bottom} = The\ distance\ between\ the\ centres\ of\ the\ current\ cell\ and\ its\ bottom\ neighbour\ [m]$

Note: The above distances is the absolute values. The distances are computed by averaging the appropriate dimension of the two cells in question.

To simplify the resulting equation each term is multiplied with the cell volume.

$V = \Delta x_{Cell} \times \Delta y_{Cell} \times \Delta z_{Cell}\ [m^3]$

The specific enthalpy rate term becomes:

Equation 7: Simplification of enthalpy rate

$$\frac{h(T_t) - h(T_{t-\Delta t})}{\Delta t} \times V$$

The specific power generation term becomes:

Equation 8:Simplification of specific heat generation

$$\frac{\dot{Q}}{m} \times V = \frac{\dot{Q}}{\rho}$$

The conduction terms become:

Equation 9: Simplification of the eastern boundary conduction term

$$\frac{\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta x_{East} \times \Delta x_{Cell}} \times V = \frac{\Delta y_{Cell} \times \Delta z_{Cell}}{\Delta x_{East}}\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{East}\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Equation 10: Simplification of the western boundary conduction term

$$-\frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{West}\right]}{\Delta x_{West} \times \Delta x_{Cell}} \times V = \frac{\Delta y_{Cell} \times \Delta z_{Cell}}{\Delta x_{West}}\left[\left(\frac{k}{\rho}T\right)_{West} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{West}\left[\left(\frac{k}{\rho}T\right)_{West} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Equation 11:Simplification of the northern boundary conduction term

$$\frac{\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta y_{North} \times \Delta y_{Cell}} \times V = \frac{\Delta x_{Cell} \times \Delta z_{Cell}}{\Delta y_{North}}\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{North}\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Equation 12: Simplification of the southern boundary conduction term

$$-\frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{South}\right]}{\Delta y_{South} \times \Delta y_{Cell}} \times V = \frac{\Delta x_{Cell} \times \Delta z_{Cell}}{\Delta y_{South}}\left[\left(\frac{k}{\rho}T\right)_{South} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{South}\left[\left(\frac{k}{\rho}T\right)_{South} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Equation 13: Simplification of the top boundary condition

$$\frac{\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Current}\right]}{\Delta z_{Top} \times \Delta z_{Cell}} \times V = \frac{\Delta x_{Cell} \times \Delta y_{Cell}}{\Delta z_{Top}}\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{Top}\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Equation 14: Simplification of the bottom boundary conduction term

$$-\frac{\left[\left(\frac{k}{\rho}T\right)_{Current} - \left(\frac{k}{\rho}T\right)_{Bottom}\right]}{\Delta z_{Bottom} \times \Delta z_{Cell}} \times V = \frac{\Delta x_{Cell} \times \Delta y_{Cell}}{\Delta z_{Bottom}}\left[\left(\frac{k}{\rho}T\right)_{Bottom} - \left(\frac{k}{\rho}T\right)_{Current}\right] = L_{Bottom}\left[\left(\frac{k}{\rho}T\right)_{Bottom} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

Note: For Equation 10, Equation 12 and Equation 14 the sign was included in the simplification and all of the conduction terms are now in a similar format e.g. The characteristic length multiplied by the difference between the conduction potentials of the adjacent cell and the current cell.

Where:

$L_{Subscript}$ = The characteristic conduction length between the current cell and the neighbour indicated to by the subscript = The area of the boundary touching the neighbour divided by the length between the cell centres $[m]$

Combined this gives:

Equation 15: Discretized transient conduction equation

$$\frac{h(T_t) - h(T_{t-\Delta t})}{\Delta t} \times V = \frac{\dot{Q}}{\rho} +$$

$$L_{East}\left[\left(\frac{k}{\rho}T\right)_{East} - \left(\frac{k}{\rho}T\right)_{Current}\right] + L_{West}\left[\left(\frac{k}{\rho}T\right)_{West} - \left(\frac{k}{\rho}T\right)_{Current}\right] +$$

$$L_{North}\left[\left(\frac{k}{\rho}T\right)_{North} - \left(\frac{k}{\rho}T\right)_{Current}\right] + L_{South}\left[\left(\frac{k}{\rho}T\right)_{South} - \left(\frac{k}{\rho}T\right)_{Current}\right] +$$

$$L_{Top}\left[\left(\frac{k}{\rho}T\right)_{Top} - \left(\frac{k}{\rho}T\right)_{Current}\right] + L_{Bottom}\left[\left(\frac{k}{\rho}T\right)_{Bottom} - \left(\frac{k}{\rho}T\right)_{Current}\right]$$

This equation is also a lot more intuitive than the differential equation. It can be interpreted the following way: The rate of change of enthalpy in the cell is equal to the sum of the heat conduction rates, into the cell, through all of the cell boundaries (East, West, North, South, Top and Bottom) summed with the power generated from within the cell.

Phase Change

For the current iteration of the model, it was assumed that only the specific enthalpy of the material will be affected by a phase change. This was done because the value of accurately measuring all the material properties of the different mixtures was deemed not worth overcoming the considerable challenge that is the extreme temperature in the furnace.

For a single-phase model, the specific enthalpy is modelled by the equation $h(T) = C_P T$. This has the desirable property that the specific enthalpy has a linear relation to temperature. A naïve approach would be to simply replace the specific heat with a piecewise function with two regions, one for solid and one for liquid. Such that

Equation 16: Naive definition of specific heat for a two-phase material

$$C_P(T) = \begin{cases} C_{P\,Solid} & T \le T_{Melt} \\ C_{P\,Liquid} & T_{Melt} < T \end{cases}$$

This however has a couple of problems, the most obvious being that the phase transition is not implicitly modelled. It should be possible to add an extra term for the phase change, to the overall equation. However, it was decided to model the phase change not as a constant temperature process but rather a process that has a very high specific heat over a small temperature range. In this case the specific heat becomes:

Equation 17: Specific heat of a two-phase material

$$C_P(T) = \begin{cases} C_{P\,Solid} & T \le T_{melt} - x \\ \dfrac{H_{sf}}{x} & T_{melt} - x < T \le T_{melt} \\ C_{P\,Liquid} & T_{melt} < T \end{cases}$$

This method sacrifices a small amount of precision but since the material properties are only estimates this was deemed inconsequential. There is however a second issue. $h(T) \neq C_P T \; but \; rather \; h(T) = \int_0^T C_p \, d\theta$. Since the specific heat is not constant the specific enthalpy becomes:

Equation 18: Specific enthalpy of a two-phase material

$$h(T) = \begin{cases} C_{p_{Solid}} T & T \leq T_{melt} - x \\ \dfrac{H_{sf}}{x}(T - x) + C_{p_{Solid}}(T_{melt} - x) & T_{melt} - x < T \leq T_{melt} \\ C_{p_{Liquid}}(T - T_{melt}) + H_{sf} + C_{p_{Solid}}(T_{melt} - x) & T_{melt} < T \end{cases}$$

This is unfortunately more complex than simply multiplying the temperature with the specific heat. However, a discerning person will notice that the specific enthalpy is still a linear function of temperature. The equation can be rewritten to make this clear.

Equation 19: Linear equation for specific enthalpy of a two-phase material

$$h(T) = \begin{cases} C_{p_{Solid}} \times T & - & 0 & T \leq T_{melt} - x \\ \dfrac{H_{sf}}{x} \times T & - & (T_{melt} - x) \times \left(C_{p_{Solid}} - \dfrac{H_{sf}}{x}\right) & T_{melt} - x < T \leq T_{melt} \\ C_{p_{Liquid}} \times T & - & T_{melt} \times \left(C_{p_{Solid}} - C_{p_{Liquid}}\right) - xC_{p_{Solid}} + H_{sf} & T_{melt} < T \end{cases}$$

In fact, Equation 19 can be rewritten in the form:

Equation 20: Modelling equation for specific enthalpy of a two-phase material

$$h(T) = C_P(T) \times T - h_{err}(T)$$

Where:

$C_P(T) =$ Equation 17

Equation 21: Residual term for calculating the specific enthalpy of a two-phase material

$$h_{err}(T) = \begin{cases} 0 & T \leq T_{melt} - x \\ (T_{melt} - x) \times \left(C_{p_{Solid}} - \dfrac{H_{sf}}{x}\right) & T_{melt} - x < T \leq T_{melt} \\ T_{melt} \times \left(C_{p_{Solid}} - C_{p_{Liquid}}\right) + xC_{p_{Solid}} - H_{sf} & T_{melt} < T \end{cases}$$

Boundary Conditions

It was decided to use a convection boundary condition $\dot{Q} = h \times A \times (T_\infty - T_{Wall})$ as the two parameters ($h \text{ and } T_\infty$) is easily controllable to mimic a plethora of other boundary conditions.

In order to accurately determine the heat flux over the boundary irrespective of cell size the following approximation of the problem was used to determine the heat flux from outside the model.

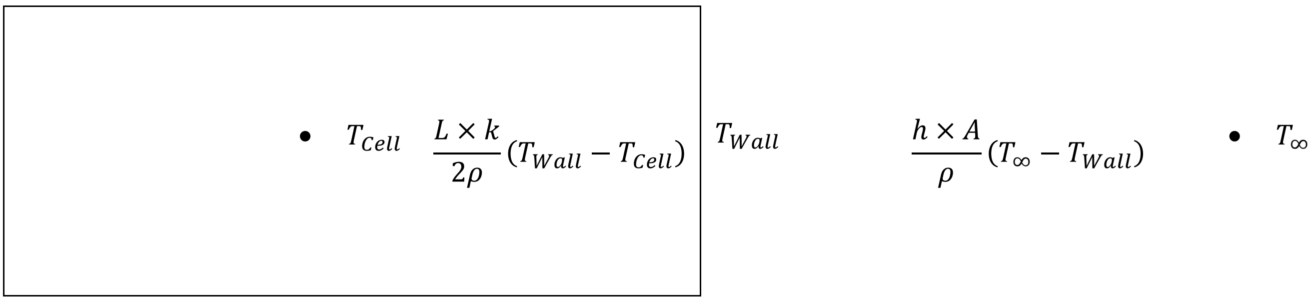

Figure 1: Boundary condition diagram

Note: The convection heat flux was divided by density to match the units of Equation 15.

The resistance analogue method was used:

Equation 22: Heat transfer from the environment to the boundary wall

$$\dot{Q}_{\infty \text{ to } Wall} = \frac{h \times A}{\rho}(T_\infty - T_{Wall}) = \frac{1}{R_{\infty \text{ to } Wall}}(T_\infty - T_{Wall}) \therefore$$

$$R_{\infty\ to\ Wall} = \frac{\rho}{h \times A}$$

Equation 23: Heat conduction from the boundary wall to the cell

$$\dot{Q}_{Wall\ to\ Cell} = \frac{L \times k}{2\rho}(T_{Wall} - T_{Cell}) = \frac{1}{R_{Wall\ to\ Cell}}(T_{Wall} - T_{Cell}) \therefore$$

$$R_{Wall\ to\ Cell} = \frac{2\rho}{L \times k}$$

Equation 24: Heat transfer from the environment to the cell

$$R_{\infty\ to\ Cell} = R_{\infty\ to\ Wall} + R_{Wall\ to\ Cell} = \frac{\rho}{h \times A} + \frac{2\rho}{L \times k}$$

$$R_{\infty\ to\ Cell} \times h \times A \times L \times k = \rho \times [L \times k + 2 \times h \times A]$$

$$R_{\infty\ to\ Cell} = \frac{\rho \times [L \times k + 2 \times h \times A]}{h \times V \times k}$$

$$\dot{Q}_{\infty\ to\ Cell} = \frac{1}{R_{\infty\ to\ Cell}}(T_{\infty} - T_{Cell})$$

Equation 25: Boundary condition heat transfer

$$\dot{Q}_{\infty\ to\ Cell} = \frac{h \times V \times k}{\rho \times [L \times k + 2 \times h \times A]}(T_{\infty} - T_{Cell})$$

Where:

$h = The\ heat\ transfer\ coeficient\ \left[\frac{W}{m^2K}\right]$

$V = The\ volume\ of\ the\ cell\ [m^3]$

$k = The\ conduction\ coeficient\ \left[\frac{W}{mK}\right]$

$\rho = The\ density\ \left[\frac{kg}{m^3}\right]$

$L = Twice\ the\ length\ from\ the\ boundary\ to\ the\ cell\ centre\ [m]$

$A = The\ area\ of\ the\ boundary\ [m^2]$

In theory this should remove any errors due to different cell sizes. In practice numerical errors may still be present.

Implementation Overview

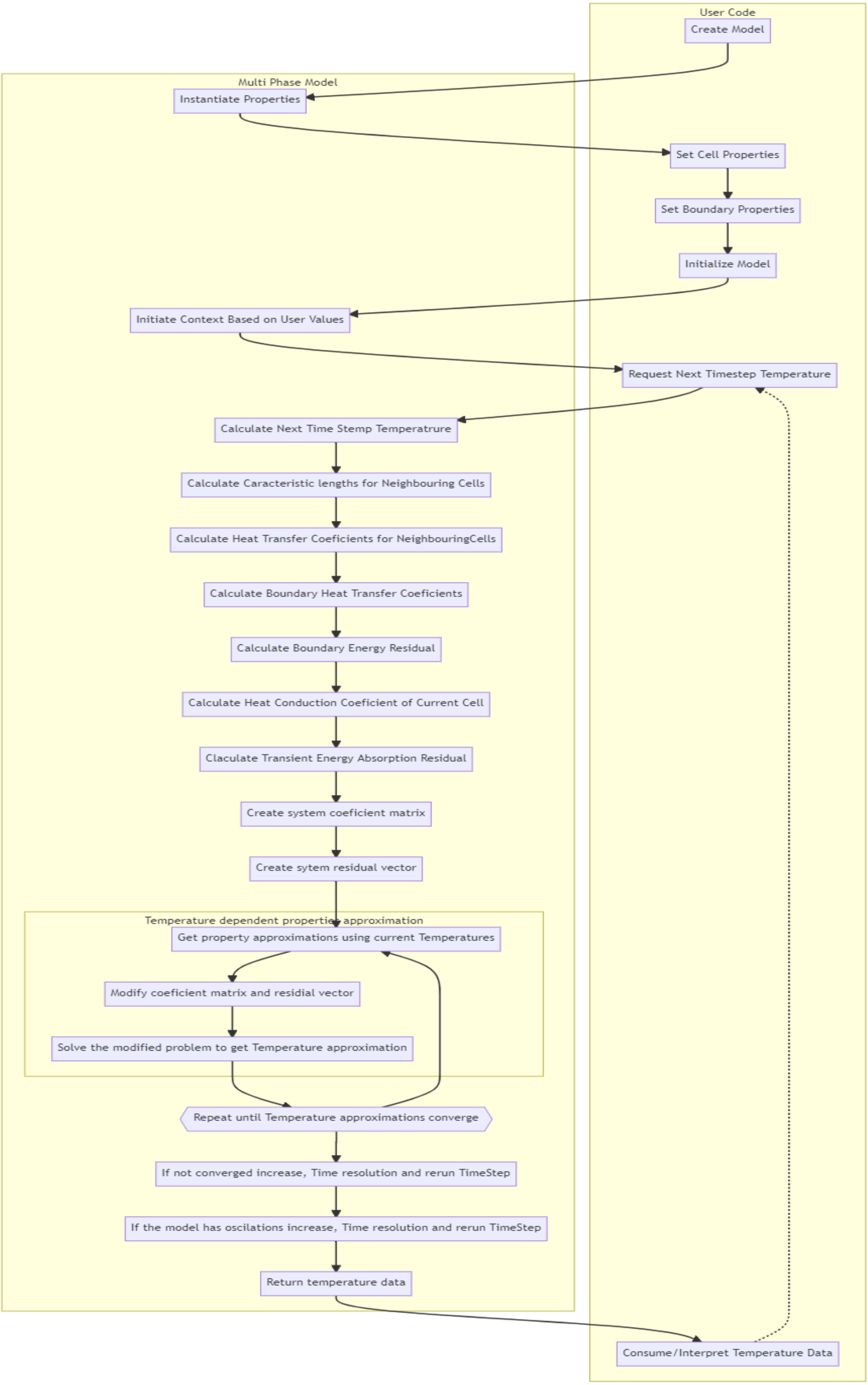

Figure 2: Model implementation overview

Results

To test the phase change element of the model a single cell was used to model an ice cube [1cm x 1cm x 1cm] in 80 °C water. Notice the 2°C transition area of the phase change.

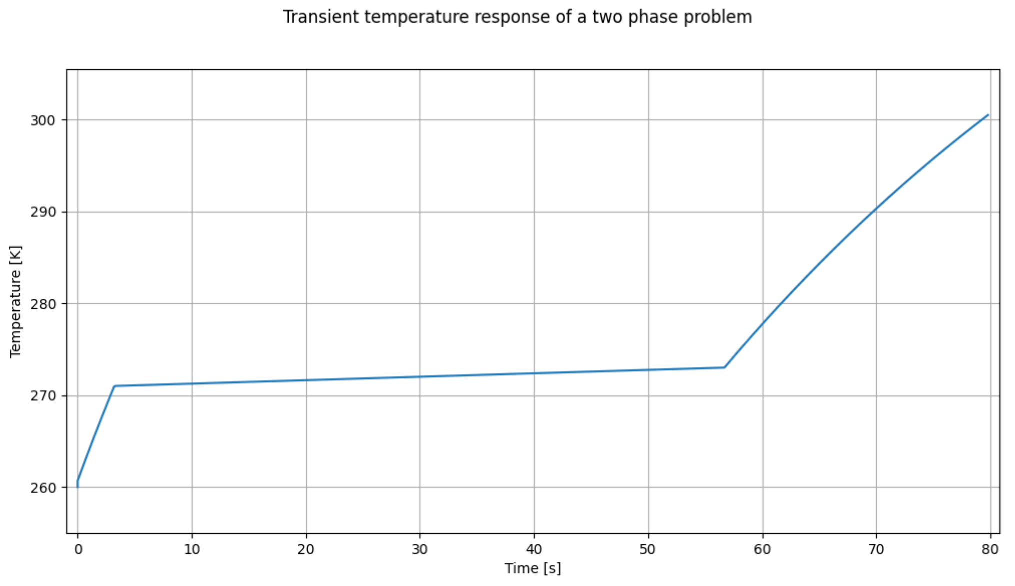

Figure 3: Single cell transient simulation

In order to test the sensitivity of the model different numbers of cells were used to model an ice rod [10 cm x 1 cm x 1 cm] which is being heated in the middle with 20 W. All sides were modelled to be perfectly insulated for this simulation.

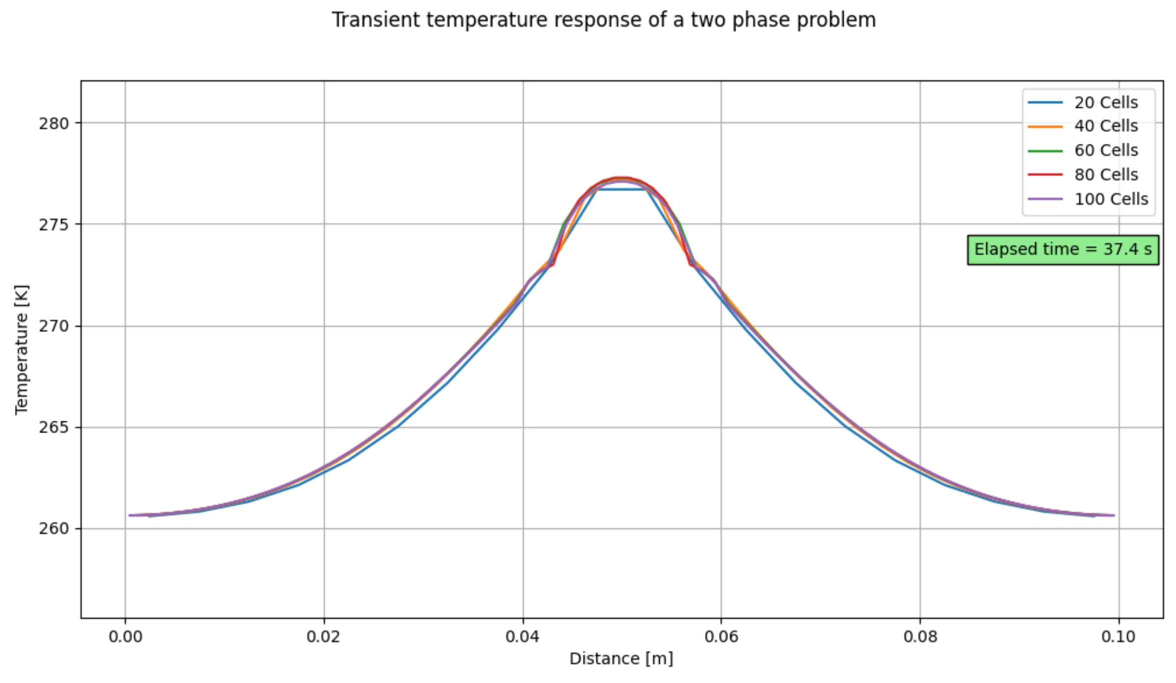

Figure 4: Variable cell transient simulation

As can be seen in Figure 4. The model is surprisingly stable even for small cell counts. Taking a closer look at Figure 5: Enlarged view of phase transition area it can be seen that this holds true even when focussing on complex areas of the graph.

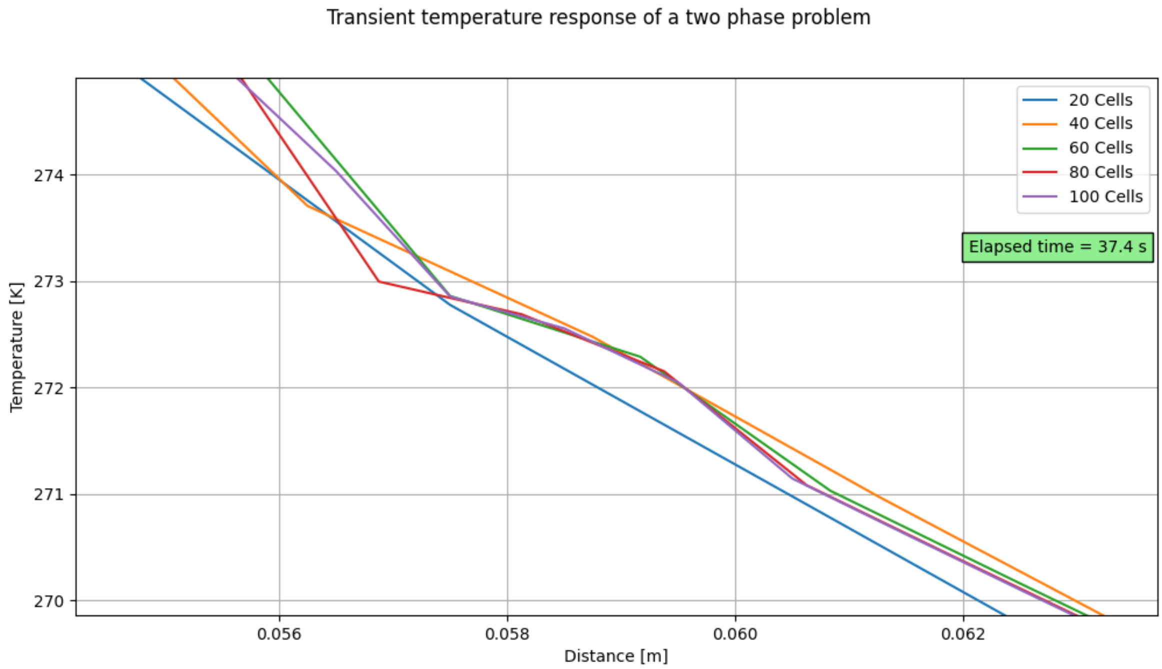

Figure 5: Enlarged view of phase transition area

In order to show the effect of numerical accuracy of the boundary condition, the ice rod model was used again. For this simulation there was no internal heat generation, and all of the sides was again perfectly insulated, except for the left side. The left side was exposed to an environment at 360 K with an exaggerated heat transfer coefficient of $100\,\frac{W}{m^2K}$.

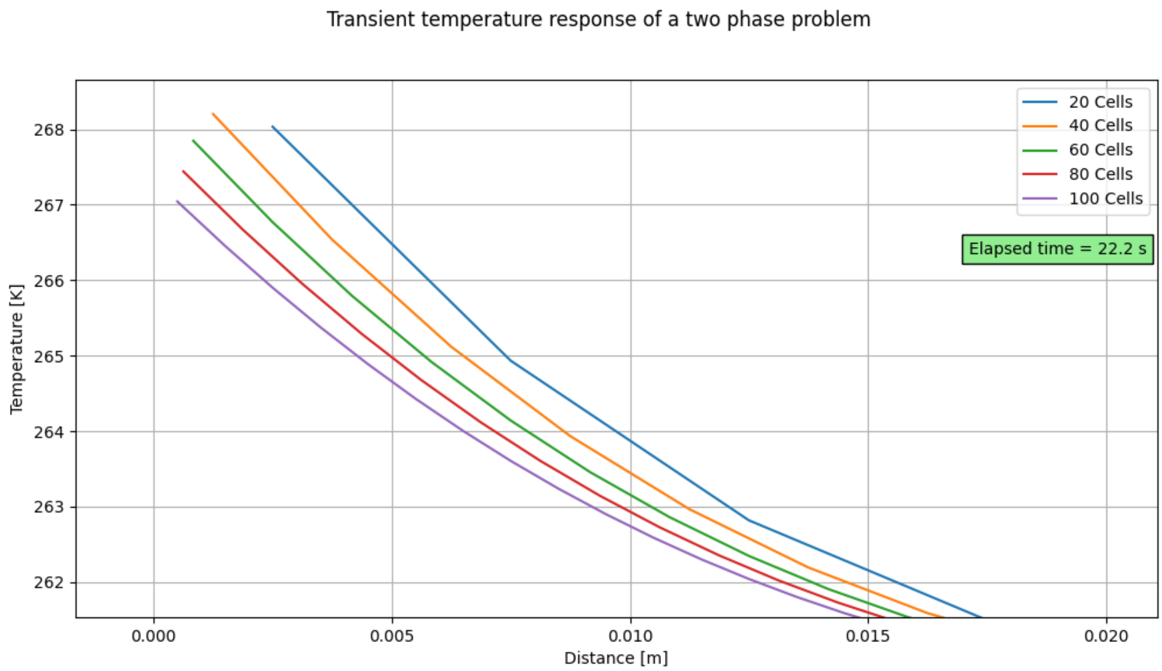

Figure 6: Boundary accuracy

References

H.K Versteeg, W Malalasekera. 2007. *An introduction to computational fluid dynamics. The finite volume method.* Pearson.