Simplified 2D Transient Heat Transfer Simulation Using Gauss Error Function and FDM

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Abstract

This Article documents the methodology used to compile a transient heat transfer simulation with the goal of calculating the time to full solidification or any specified temperature of a metal casting, this simulation may serves as a confirmation of Chvorinov's rule, furthermore the simulation will identify the heat transfer topography, allowing the user to identify the location of possible solidification errors, however for the purpose of simplification, only the liquid phase cooling of pure iron will be considered in this report. Euler methods will be discussed with special attention paid to explicit forward approximation and how Gaussian error can be used to simplify the simulation, in an attempt to reduce processing time. A look at the advantages and disadvantages of using this method will be considered and explanations given the decisions taken in the methodology of the simulation, the use of software will be discussed. The article will conclude with a look at the other applications for this simulation as well as the limits of this simulation.

Keywords: Euler, solidification, Chvorinov, Gauss-error, simulation.

1. Introduction

Finite Difference Methods (FDM) are amongst the oldest and simplest methods for solving differential equations [5], which when combined with more complex mathematics and a user interface are packaged and sold to foundries in the form of Magmasoft, Flow3D or any of a number of excellent simulation packages. However the cost of many of these packages and non-technical nature of these software packages make them inadequate to conduct numerical experiments on an academic level. On the other side of this argument, one could say that it is not realistic to expect a degree level engineer or foundry technician to write a program in FORTRAN or C++ to analyse a real world heat transfer

and solidification problem. This report aims to find a middle ground between the Doctorate mathematician and engineering student, where an accurate FDM model can be setup without the need to learn a new programming language.

Chvorinov's rule calculates time to solidification of a casting based on the mold constant, volume of casting and surface area of casting [4], this report will discuss how an FDM simulation may provide additional info. It is possible to represent a 3D object in 2D by using a symmetrical through the object and dividing this into a mesh (trial and error allows the user to balance accuracy of the system with computational requirements by adjusting the size of this mesh) however there is a saturation point where the mesh will insignificantly improve accuracy with a significant increase in processing time [1]. To highlight this, the article will first consider

the theory behind the simulation and setting up of the simulation. Microsoft Excel, is a widely used software package capable of non-linear mathematics, able to run loops for solving complex systems or differential equations and presenting results graphically without the need for a post-processor the simulation will show how using an explicit approach each result is output to the next time step where the same forward approximation is applied and so on, until the pre-defined time is reached, or model is solidified. The simulation model may be downloaded from: https://drive.google.com/file/d/0B5C8Alae_Y21VDc5YlVTREZi VGM/edit?usp=sharing.

Finally conclusions about the results will be drawn and the accuracy of the results evaluated before final remarks and conclusions are made.

2. Theory

Two separate but equally important areas were used to create this simulation, these were: Transient heat transfer theory and explicit Finite difference theorems.

2.1. Transient Heat Theory

The Biot number is a dimensionless relation between conduction through a body and convection at the surface of that body. It can be viewed as a criterion for heat transfer [3]. A Biot number of less than 0.1 may be modelled by simple lumped capacitance model [6]. A Biot number greater than 0.1 indicates that heat gradients occur within the body and hence more complicated transient heat equations are required to evaluate such a system.

$$Bi = \frac{hV}{kA} \tag{1}$$

(Bi) Biot Number, (h) heat transfer coefficient, (V) volume of body, (k) thermal conductivity, (A) body surface area.

Fig. *1* shows a generalized solidification curve of a pure metal, transient heat transfer in metal [8] solidification must incorporate 3 stages, liquid, mushy & solid. In a pure metal, latent heating remains at a constant temperature, in reality this is seldom the case the diagram also ignores undercooling. For the purpose of simplifying this report the afore mentioned factors will not be included in the methodology.

2.2. Finite difference method

Fourier heat laws and integration of this law into various forms of heat transfer has been covered extensively in literature, to maintain simplicity the author will focus only on the applied formula. By looking at each mesh cell as a semi-infinite solid, one may use formula (2) [7], applying Laplace transforms results in formula (3) which provides the user with a temperature change in the cell over a certain number of time-steps. Small cells sizes and shorter time-steps provide more accurate results however large models are processor intensive and a balance should be found between accuracy and simulation time.

$$\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right) = \frac{1}{\alpha}\left(\frac{\partial T}{\partial t}\right) \tag{2}$$

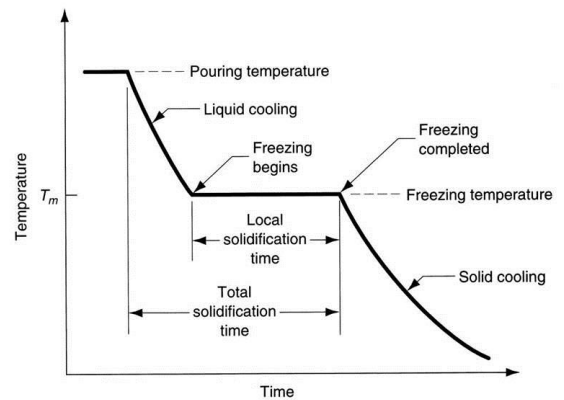Fig. 1. Typical coolling curve for metal solidification, neglecting undercooling [8]

$$T(x,t) = T_0 \text{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) \tag{3}$$

$$\frac{T-T_0}{T_1-T_0} = 1 - \frac{2}{\sqrt{\pi}}\int_0^{\frac{x}{2\sqrt{\alpha t}}} e^{-s^2} ds \tag{4}$$

$$\alpha = \frac{k}{c_p\rho} \tag{5}$$

where s = $\frac{x}{2\sqrt{\alpha t}}$, argument of error function erf

Thermal diffusivity (α) is the result of thermal conductivity (k), specific heat (c_p) and density (ρ). Each cell is subject to the following initial conditions at the beginning of each time step.

$$T(x,0) = T_0$$
$$T(x,t) = T_1$$
$$T(x \rightarrow \infty, t) = T_0$$

Fig. 2. Initial boundary conditions which will be considered with equation 3

Specific heat varies according to melt temperature, while the author will only consider specific heat in the liquid phase, if it is important to understand that this plays a significant role in calculating time for full solidification, where latent heating is considered (See specific heat range below for liquid, mushy and solid phases).

$$c(T) = \begin{cases} c_L & T_1 > T_L \\ Cp + \dfrac{Q}{T_L - T_s} & T_s \leq T_1 \leq T_L \\ c_s & T_s < T_1 \end{cases}$$

The change in temperature is considered in a 2D plane, hence x and y vectors are considered separately and consolidated using an FDM star node method i.e. each node expresses the average temperature of a cell, this temperature is a function of the average temperatures of the four nodes adjacent to it, these four nodes are in turn are effected by the 4

nodes adjacent to each of them. This redundancy is addressed by systematic dumping of time-step results, this will be explained in the methodology.
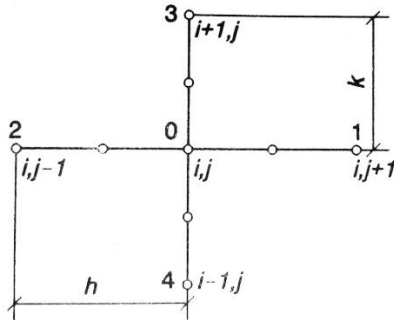

Fig. 3. Star configuration, points 1,2,3,4 represent the cell temperature of adjacent cells [7]

Boundary conditions are also considered the interface between the metal and mold for example alters the heat profile as the metal cools the mold wall will increase in temperature, however the boundary temperature will not stagnate at a median between the mold and melt initial temperatures but rather once the temperature gradients has stabilized the overall temperature will continue to decrease until ambient temperature is reached within the mold and melt.

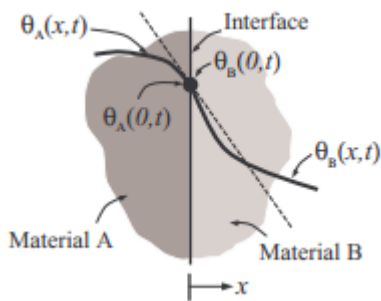$$Ts = \frac{m_A T_A + m_B T_B}{m_A + m_B}$$

$$m = \sqrt{kpCp}$$

Fig. 4. Temperature gradient between melt and mold, the interface point changes in the y direction also over time [2]

3. Simulation

As expressed earlier, Microsoft Excel will be used to solve this example problem due to its general availability, this report uses Microsoft Office 2013, any version may be used however it must be noted that versions older than 2010 do not include the error function (erf) as part of its solver.

A 275x275 mesh was drawn, with a cell size of 2mmx2mm. Cells are separated into 4 sections, melt, boundary, insulation and mold. Eleven separate sheets are used to describe the problem these were "DATA", this includes all material properties for the mold, insulation and melt. The "DIM" sheet separates the mesh into distinct parts by assigning a number to each part (Melt = 1, Boundary = 2, and so on) this sheets is used to ensure that each cell type uses the correct formula during simulation. "INITIAL" sets the starting temperature of the simulation, these values are set in the "DATA" sheet and determine the pouring temperature & ambient temperature.
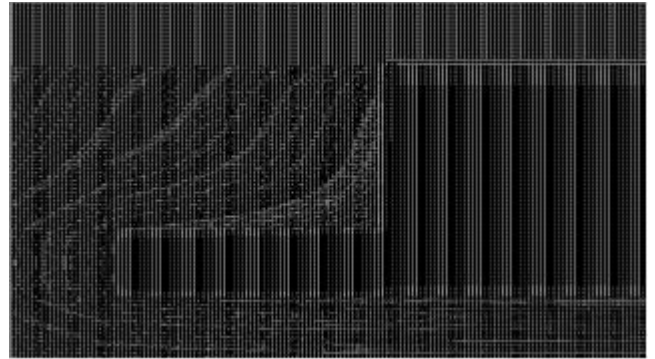

Fig. 5. High density mesh view of model, the right side may be considered symmetric thus the mesh count may be halved and appropriate mirrored boundary conditions added the right most cells

To run a simulation in excel a MACRO is required which loops the equation through the time-steps, the "DUMP" sheet is used to address redundancy of the calculated, i.e. a solution cannot be used as input data in the same formula used to calculate it (see Fig. 6). A macro script (see linked simulation spreadsheet) specifies the cell co-ordinates for the simulation, dumps the results to the "DUMP" sheet, updates "AVE" visualization sheet & runs each timestep concurrent to one another immediately after the all sheet calculations are complete.
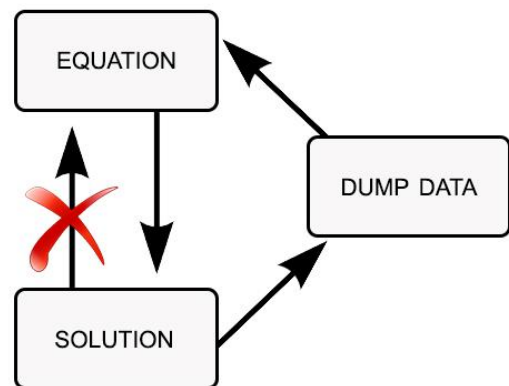

Fig. 6. Graphical representation of how redundancy is overcome using "dump data"

Formula (3) is then applied in 4 directions in the sheets "T(x,t) +", "T(x,t)−", "T(y,t) +" & "T(y,t)−" before "AVE" sheet applies the 5 point node (see Fig. 3) to calculate the average temperature of the node, these results are then added to the "DUMP" sheet as T_0, i.e. acts as a new initial

temperature for the time-step. Using this approach, Fourier number, heat transfer distance (x value in "DATA") and thermal diffusivity remain constant thus the error remains constant for all time steps during heat transfer in the liquid phase. For simplicity specific heat of iron (used in this example) remains constant above 900°C and changes are viewed as being insignificant.

The "AVE" sheet consolidates all information. Adding conditional formatting to the sheet with a colour scale visualizes temperature gradients, Microsoft Excel is also able to give the user a visualization of the problem. Running the "start" macro begins the simulation.
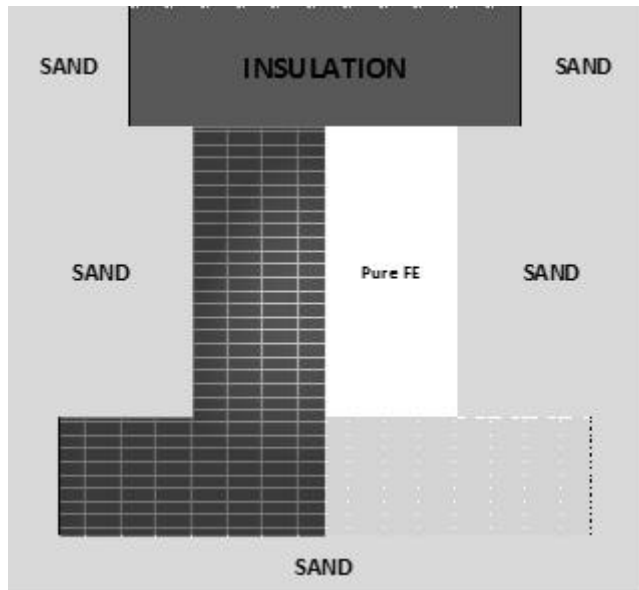
Fig. 7. Conditional formating illustrates temperature gradient changes after each time-step

The simulation may be downloaded from: https://drive.google.com/file/d/0B5C8Alae_Y21VDc5YlVTREZiVG M/edit?usp=sharing as a free template for transient heat modelling.

4. General remarks & Conclusion

The purpose of this report was to simplify 2D heat transfer using a simple finite difference method and applying this to a 2D mesh. The article describes the general methodology behind applying this theory to Microsoft Excel, a link to the spreadsheet can be found below. As explained above this article only sets out to lay the foundation for 2D transient heat transfer simulation, the addition of latent heat and variable specific heat into the governing formulas will increase accuracy and will allow a full solidification model to be completed.

In future the author would like to add volume change to the simulation, this will allow the user to see cavitation and riser funnelling. However this can all be added by future users for a more accurate model.

5. Acknowledgements

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