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Numerical Simulation on Heat Transfer Analysis in Zinc Solidification Process Using Enthalpy Porosity Method

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Abstract: *The solidification study of metal alloys are very common than that of pure metal. The research article presented focused on solidification of pure zinc. The simulations are conducted using Volume of fluid and enthalpy porosity model. This fixed grid method considered is applicable to both pure and metal alloys. The effects of heat transfer analysis during solidification of molten zinc with different thermal boundary conditions are studied. The contours show the location of solid-liquid interface and metal-air interface with time. The transient study of melt fraction and heat flux for different thermal boundary conditions presented to explain the heat transfer analysis with phase change. The simulation also shows the shrinkage of the solidphase after completion of the solidification process.*

Keywords: Pure zinc, enthalpy-porosity model, solidification, rectangular cavity.

I. INTRODUCTION

Zinc is one of the important non-ferrous metals. It is being used in a variety of industries and products. Pure zinc is predominantly used as a coating material for corrosion resistance. Zinc is also used for many industrial alloys. Zinc in various forms is used in cosmetics, paints, inks, soaps, pharmaceuticals, plastics, electrical equipment, batteries, and textiles. Zinc is also used as a casting material for various metal products. It is therefore important to understand the melting and solidification process of zinc. The numerical and experimental studies on melting and solidification are available for different phase change materials (PCMs) likeinorganic, organic PCMs, pure and alloys substances. Some of the PCMs have high phase change temperature and some have a low melting temperature. The solidification studies are also considered for different casting processes. A large amount of heat is transferred as latent heat in the phase change process which affects the macroscopic behaviour of the substance. In this study**,** solidification of zinc is simulated using enthalpy porosity model. The volume of fluid (VOF) is incorporated with the enthalpy porosity model to define the PCM and air interface at the open surface.

Bermudez and Otero compared the solidification of aluminium slab using direct chill casting and electromagnetic casting processes. The limitation of the proposed numerical model is a fixed grid method(A. Bermudez, 2006). Chakraborty studied the solidification of pure substance water using enthalpy porosity model(Chakraborty, 2017). The study considered the variation in specific heat in both the phase and showed a good agreement with the prediction made by Kowalewski and Rebow(Rebow, 1999). Bot and Arquis simulated the one dimensional model of deposition and solidification of successive metal layers on a cold surface(Cedric Le Bot, 2009). The model used for simulation not considered the convective phenomena because of negligible flow time.

Tianet. al studied the effect of cooling rate in polymorph selection during solidification of zinc(Ze-an TIAN, 2015). The study showed the effect of polymorph selection is different at a different stage of cooling. Wenyi Hu optimized the casting of AZ31 magnesium slab using the direct chill method with different cooling speed (Wenyi Hu, 2013). Solidification studies are presented for different metals and alloys like Nickel (B.T. Bassler, 2003), tin(Hwang, 1997) etc. Tomasz and Ewa simulated the solidification of Copper using finite element method. They used a front tracking method to locate the solid-liquid interface(Tomasz Skrzypczak, 2012). Similar numerical studies are also presented by several authors with different boundary conditions (Slota, 2011; Zabaras N, 1990; N. T. Zabaras N, 1995; R. Y. Zabaras N, 1989). Lewis and Ravindran simulated filling and solidification of molten aluminium in spiral and spillage wheel type cavity(R. W. Lewis, 2000). They used the finite element method with a fixed grid for the solidification study. Fixed grid method is advantageous over the moving grid. Fixed grid considers the total materials as a single phase and for moving grid the control volume is treated as two-phase. In the case of alloys,a number of materials are present and using moving grid the calculation is complicated. In such a situation, the fixed grid method is more effective. During the casting of metals, the impurities are always present in an optimum amount and fixed grid method is appropriate in such cases. Literature survey shows that there are very few literatures available on solidification of pure metal. The study of phase change for pure metals is important to set a benchmark for alloys. The difference in the thermal behaviour of metal and alloys can be studied by performing this type of simulation.

In this paper, the authors focused on the fixed grid method for simulation of solidification of pure zinc under different thermal boundary conditions. Volume of fluid (VOF) method is used to describe the interface of air and zinc and enthalpy porosity model is adapted to locate the solid-liquid interface of the phase changing material. The proposed model is widely applicable to different thermal boundary conditions as well as different inorganic/organic PCMs, high/low phase change temperature materials. The effect of the convection heat transfer coefficient on the solidification process and time are compared.The solidification of zinc presented in this research paper, studied the effect of convection heat transfer coefficient on solidification time.

II. MATHEMATICAL MODEL AND COMPUTATIONAL MODEL

Phase-change processes come under the moving boundary problem. The change in density due to cooling and phase change, the velocity suppression occur which results in an irregular interface. An axisymmetric rectangular cavity has been taken to the study of solidification process of molten zinc. The size of the cavity is 28mm×78mm. The size of the cavity is very small in order to minimize the computation time. The cavity is filled with molten zinc. The schematic diagram of the cavity is shown in figure 1. The initial temperature of molten zinc is 4.5 degrees higher than that of mean solidification temperature. The study has been performed for different convection heat transfer coefficient. The cavity is exposed to air during the solidification process. The thermo-physical properties of molten zinc are chosen as commercially available zinc. The density of solid zinc is 7134 kg/m^3 and 6927 kg/m^3 for liquid zinc, specific heat 900.1 J/kg.K, thermal conductivity 164W/m.K, viscosity is 0.00358 kg/m.s, latent heat 109kJ/kg, solidus temperature is 693K and liquidus temperature is 698K. Ansys-fluent16.2 is considered for simulation of the casting process. VOF model has been used to describe the zinc-air system with a moving internal surface and no inter penetration of two media (air and zinc). Enthalpy-porosity model is used to identify the solid-liquid interface in the phase change region. The enthalpy-porosity method is used to describe the velocity suppression in solid phase (Sin Kim, 2001). The governing equations of fixed grid enthalpy model are satisfied by of solid and liquid phase of phase changing material. The no-slip boundary condition is maintained at the walls. Axisymmetric, laminar, and incompressible flow within the cavity is assumed during the simulation process. The thermo-physical properties like thermal conductivity, specific heat, the viscosity of zinc are assumed to be constant with temperature. The density of zinc is only varying during phase transition. The momentum source term is used to describe the movement through the porous medium, at the solid-liquid interface. The value of the mushy zone constant is taken as 10^5 (A.D. Brent, 1988).

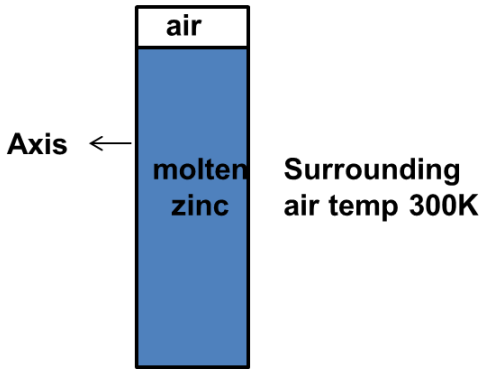

Figure 1: Schematic diagram of computational domain

The governing equations used to explain the solidification phenomena are

Continuity equation:

$$\frac{\partial \alpha}{\partial t} + u_i \frac{\partial \alpha}{\partial x_i} = 0 \qquad (1)$$

In the above Eqn. 1 the volume fraction of secondary material PCM or zinc is denoted by α. The value of α is one at solid/liquid zinc interface and at the zinc-air interface, the value of α lies between zero and one. The volume fraction in eqn. 1 will only solve for the secondary phase (zinc) and the primary-phase volume fraction will be computed based on the following constraint

$$\alpha_{air} = 1 - \alpha \quad (2)$$

It is important to mention that the continuity equation, momentum balance and energy balance equation are applicable for both solid and liquid phase of zinc.

Momentum balance equation:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_i}(\rho u_j u_i) = \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{\partial p}{\partial x_j} + (\rho - \rho_{ref})g + S_i \quad (3)$$

ρ_{ref} is the density of cell calculated at the reference temperature T_{ref}.

Energy balance equation:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) \quad (4)$$

ρ, k and μ denote the density, thermal conductivity and dynamic viscosity of molten zinc and air mixture respectively (Debasree Ghosh 2019). The momentum source term is S_i, u_i is the component of velocity along cartesian coordinate x_i , and the specific enthalpy of both the air and zinc respectively in the specified region is denoted by h. The Eq. 3 and Eq. 4 are valid for air, zinc and their interface.

The enthalpy is defined as$h = h_{ref} + \int_{T_{ref}}^{T} C_p dT + \gamma L$. $href$is enthalpy at temperature $T\ ref$. L is the latent-heat for solid-liquid phase change of zinc, and the liquid fraction (γ) in computational cell the during the phase transition over a range of temperatures are calculated by the following relations:

$$\left.\begin{array}{c} \gamma = 0\ at, T < T_s \\ \gamma = \frac{T - T_s}{T_l - T_s}, at T_s < T < T_l \\ and\ \gamma = 1\ at T > T_l \end{array}\right] \quad (5)$$

The source term in momentum is porosity function and defined using Carman-Kozeny equation. For flow through porous media and the source is defined as(E. Assis, 2007):

$$S_i = -C \frac{(1-\gamma)^2}{\gamma^3 + \varepsilon} u_i \quad (6)$$

C in Eqn. 6 is called mushy zone constant.

SIMPLE pressure-velocity coupling scheme is used to solved the momentum, continuity and energy equations. Discretization scheme used is second-order upwind for momentum, PRESTO for pressure, second-order upwind energy and geo-reconstruct for volume fraction. The boundary conditions are: convection heat loss at surrounding temperature 300K and the top of the cavity is open and assumed to be at atmospheric pressure. The initial temperature of the molten zinc PCM is kept at427°C which around is 4.5°C higher than the mean solidus temperature of pure zinc.

The simulation is repeated with different time step and grid independency is also checked to establish the model. The results are shown for time step 0.001sec and with minimum cells 25056. The details of grid independency study are given in Table 1. The convergence criterion is $10^{-3}$for velocity, continuity and 10^{-6} for energy. The solutions are converged in every time step. The mathematical model is solved for different convection heat transfer coefficient at the wall boundary.

Table 1: Details of grid independency study

Number of nodes	Time step (sec)	Time of solidification (sec)
50040	0.001	36
72560	0.001	36
25056	0.001	36
25056	0.0001	36
25056	0.0005	36

III. RESULTS AND DISCUSSION

The casting or solidification of pure zinc is studied for different boundary conditions. In this research article solidification of superheated zinc in a rectangular cavity are simulated. The solidus and liquidus temperature of zinc are taken at 420°C and 425°C respectively. The solidification of zinc is a very fast process. The solidification of zinc is studied experimentally and the process is very fast and except solidification time no other experimental data are recorded. Therefore, the simulation of solidification process is required for the investigation of the complete casting process.

For numerical simulation of solidification process, the initial temperature of molten zinc is taken as 427°C (700K). Figure 2 shows the solidification time required for zinc under different thermal boundary conditions. These boundary conditions are: solidification with different convection heat transfer coefficient (htc) 600 W/m^2.K at side and bottom walls, htc of 300 W/m^2.K at side and bottom walls, htc of 600 W/m^2.K at side and insulated bottom walls, htc of 300 W/m^2.K at side and insulated bottom walls, insulated bottom and constant side wall temperature (300K) and htc of 200 W/m^2.K at side and insulated bottom walls. The solidification time required is minimum for constant side and insulated bottom wall temperature (300K) and it is around 3.5

sec. The solidification time is around 36 sec (maximum) for wall convection heat transfer coefficient 200 W/m^2.K with and without bottom insulation. It is observed from Figure2 that the solidification time is not affected by the bottom insulation. The time required for solidification is same for same side wall convection heat transfer coefficient. The reason behind it is the solidification starts from both the vertical wall and the width of the cavity is less than the height or vertical wall, therefore insulated bottom wall is able to minimize the effect of the cold vertical wall. The variations of heat flux with time are not similar for all convection boundary condition. Figure 3 shows the variation of heat flux. The negative sign of heat flux represents the heat loss from the control volume or cavity. The figure concludes that the heat flux from the cavity decreases as solidification proceeds. The trend of heat flux change is almost linear for convection heat transfer coefficient 200 and 300 W/m^2.K (with and without bottom insulation) and the trend of heat flux is nonlinear for high heat transfer coefficient 600 W/m^2.K (with and without bottom insulation). The slope of heat flux curve is increasing with increase in heat transfer coefficient and slope becomes variable for higher convection heat transfer coefficient.

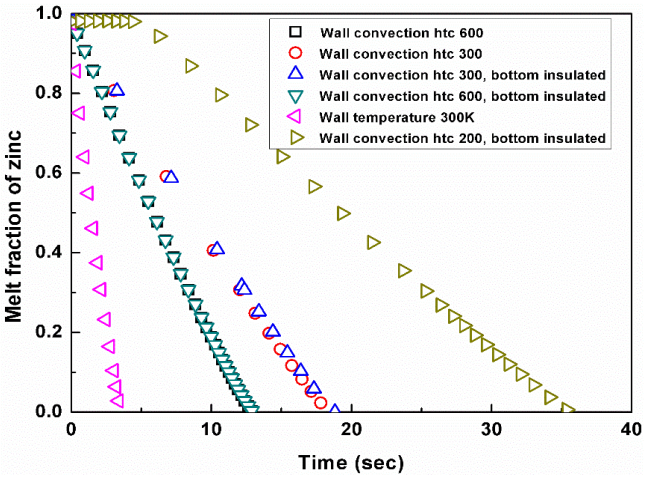

Figure 2: Melt fraction of zinc under different boundary conditions

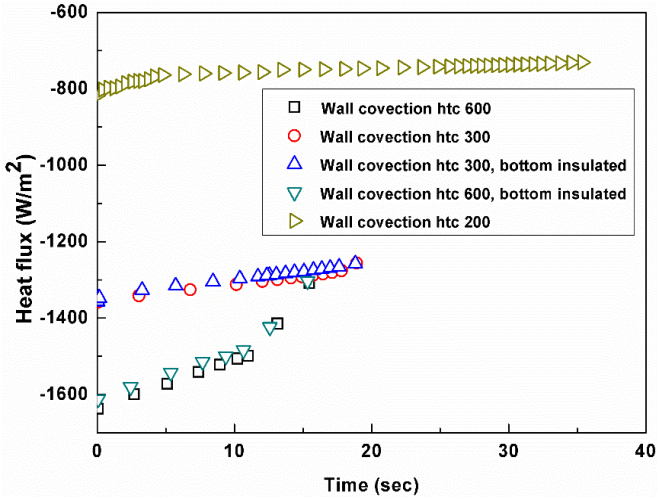

Figure 3: Heat flux variation with time for different wall convection thermal boundary condition

The contours of melt fraction with time are shown in Figure 4. The red colour represents the complete liquid phase and blue colour represents the complete solid phase. The half cavity is presented in the figure. The contours are shown for solidification with convection heat transfer coefficient (htc) 200 W/m^2.K at the side and insulated bottom walls. It is observed that solidification starts at top of side wall due to the effect of cold vertical temperature and atmospheric air present at the open top of the cavity. With time the thickness of the solid phase starts increasing from the vertical wall. The thickness of the solid phase is not uniform over the vertical wall; due to the increase in density of cold metal the thickness of solid zinc is higher in the bottom than that of the top. Towards the end of solidification, the thickness of the solid phase is minimum at the middle of the cavity and highest the bottom. After complete solidification the top surface is not observed to be linear but, a decrease in material level toward the axis of cavity is noticed. The increase in density due to solidification causes this shrinkage in volume of zinc.

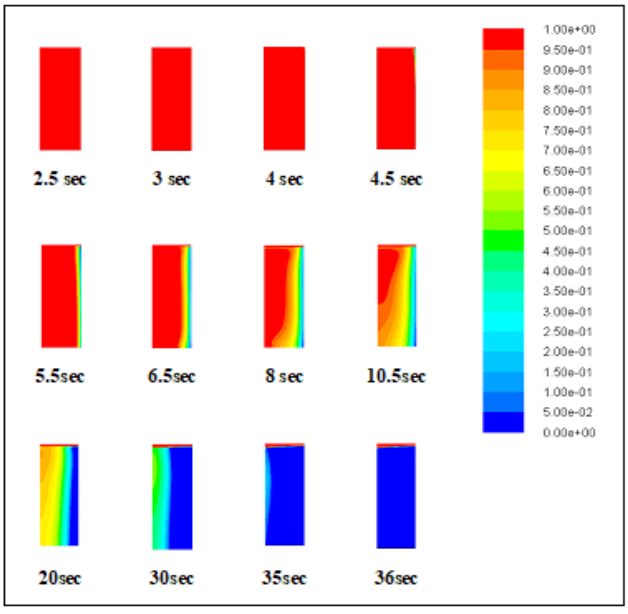

Figure 4: Contour of melt fraction of zinc in half cavity

IV. CONCLUSION

Numerical study helps to identify and analyse each step of a process. Especially for very fast processes, numerical simulations are advantageous. It is the safe and economical way of process investigation. In this article, the solidification of pure zinc is studied for different convection boundary condition. The results show that solidification process varies. The solidification of any high-temperature PCM is always very fast. The results also show that bottom insulation is not affecting the time of solidification for the same convection heat transfer coefficient (htc). The melting time is highest for lowest convection heat transfer coefficient htc (200W/m^2.K) and minimum for constant cavity wall temperature, 300K. Such studies can be extended to determine the molecular dynamics of metal. The solidification of zinc alloys can also be investigated and compared with pure zinc using this fixed grid enthalpy porosity model.

List of symbols

α	Phase volume fraction of nth fluid
u_i	Velocity component in ith direction (m/s)
x_i	Cartesian component
t	Time (s)
ρ	Density of PCM (kg/m^3)
μ	Viscosity of PCM (kg.m/s)
p	Pressure (N/m^2)
g_i	Gravitational force (m/s^2)
S_i	Momentum source (kg/m^2.s^2)
h	Enthalpy (kJ/kg)
k	Thermal conductivity (W/m.K)
T	Temperature (K)
T_w	Wall temperature of the cavity (K)
C	Mushy zone constant
γ	Liquid fraction
T_s	Solidus temperature (K)
T_l	Liquids temperature(K)

Conflict of Interest

The authors confirm that there is no conflict of interest to declare for this publication.

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