2-D Numerical Simulation of PFMS Process Considering Interfacial Heat Transfer between Melt Puddle and Rotating Drum

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Abstract: Planar flow casting process PFC (also known as single-roll melt-spinning or planar-flow melt spinning) is a rapid solidification process to produce continuous amorphous alloys strips with rapid cooling, desirably the molten metal is an alloy with a quenching rate of about $10^5$ – $10^6$ K/sec. The present work attempts to understand the transient fluid flow and heat transfer characteristics of the molten metal alloy combinations of (Fe-Si-B) and (Ni-B) and the resulting melt puddles formed on the moving substrate and thickness of the amorphous metal alloy strips. At the melt puddle and moving substrate interface, heat penetrates inside by conduction. Numerical simulation is attempted by considering 2D, unsteady fluid flow with free surface, surface tension, and heat transfer. An air pocket appears at the bottom of the melt puddle due to air ingress near upstream meniscus creating an unstable puddle which affects the smoothness of the amorphous metal alloy strip thus formed. Sliding mesh with coupled walls interface scheme between fluid-solid (puddle/roller surface) solution is employed for identifying the interfacial heat-transfer at the roller surface.

I. INTRODUCTION

Planar Flow Casting process can be clearly explained with the help of schematic shown in Fig 4. In PFC process the Fe$_{78}$Si$_9$B$_{13}$ alloy in crucible is heated above melting point by electromagnetic induction. By applying the gas pressure on the top of the crucible molten metal is forced through a nozzle slit in close proximity to the surface of the rotating copper roller. When the molten-metal impinges on the roller surface melt puddle is formed between the nozzle and the roller surface, which acts as a reservoir for ribbon formation and due to high cooling rates of $10^5$ – $10^6$ K/s molten metal solidifies rapidly within a very short period of time (in order of milliseconds) forming amorphous structure by surpassing crystallization with no latent heat release resulting in amorphous ribbon. Solidified ribbon is dragged out by the rotating roller from the melt-puddle zone. Significant amount of heat from the melt puddle is absorbed by the copper roller by conduction and a little amount of heat is transferred to air by convection. Roller surface is maintained below glass formation temperature by continuous circulation of water on the inner surface of roller.

Fig 1. Schematic drawn of Planar Flow Casting process.
II. PROBLEM DESCRIPTION AND METHODOLOGY

A. The aim of the present work is to:
   - Study the effect of thermo physical properties on the ribbon thickness value and the interfacial heat transfer between the melt-puddle and the roller surface.
   - Study the initial development of the melt-puddle, transient phenomenon of fluid flow and heat transfer characteristics in the nozzle-wheel gap and the heat transfer into the roller underneath the puddle.
   - Compare puddle shapes of two different alloys when puddle is formed and developing at same instants of time.

The domain considered for the present study is shown in Fig 2, which includes the air domain and the copper roller domain.

B. Methodology

Numerical simulation is attempted by considering 2D, unsteady fluid flow with free surface, surface tension, and heat transfer for the governing equation with related boundary conditions is solved by using computational fluid dynamics software package ANSYS WORKBENCH and FLUENT v 14 to simulate and analyses the planar flow melt spinning process.

III. NUMERICAL METHOD:

The Space of fluid domain (air and melt) between flat nozzle wall and curved cooling wheel and solid domain (copper) is considered as the computational domain. To include the surrounding atmosphere, domain is extended on both sides of the nozzle wall and is assumed to be initially filled with air as a primary phase. Upon ejection, molten metal enters the domain through nozzle slit as a secondary phase. To simulate the two phase flow, volume of fluid (VOF) technique is using an explicit with geometric reconstruction scheme is employed. Energy, continuity and momentum equations are solved with first order upwind spatial discretization.

I. Sliding Mesh Theory:

The sliding mesh model is a special case of general dynamic mesh motion where in the nodes move rigidly in a given dynamic mesh zone. Additionally, multiple cells zones are connected with each other through non-conformal interfaces. As the mesh motion is updated in time, the non-conformal interfaces are likewise updated to reflect the new positions each zone. It is important to note that the mesh motion must be prescribed such that zones linked through non-conformal interfaces remain in contact with each other (i.e., “slide” along the interface boundary) if you want fluid to be able to flow from one mesh to the other. Any portion of the interface where there is no contact is treated as a wall.
2. Geometry and grid generation:
Modeling and meshing have done by using workbench and ICEM CFD to design the geometry of the model and creating a good orthogonal quality hexa mesh of minimum value 0.8 wherein 0.99 is maximum value could be reached as the mesh shown in fig 3.

Maximum Aspect Ratio = 3.00580e+01
No of cells: 916326
No of nodes: 906700

3. How to evaluate the ribbon thickness:
2D time-dependent numerical simulations are performed to examine the effect of process parameters on puddle length (L), melt contact length (Ln) at the nozzle wall and ribbon thickness (t) using CFD software ANSYS FLUENT.

Isotherm at glass transition temperature (Tg) of the alloy is considered as the solid-melt interface. Ribbon thickness is measured as the vertical distance from the wheel surface to the point of tri-junction J*, which is a common point of three phases; air, melt and solid ribbon. In the present study, tri-junction is identified as the point of intersection of downstream meniscus of the puddle showing melt-air interface and isotherm at glass transition temperature. Puddle length is measured as the distance between the point of contact of upstream meniscus with the wheel and the position of tri-junction at the downstream on the wheel surface. Melt contact length at the nozzle (Ln), is measured as the distance between the contact points of melt on both sides of the nozzle wall. This helps to define the dimension of the nozzle walls of the copper crucible. Length of nozzle walls is taken as 4 mm each, for all the geometries in the present study. L, Ln and t are shown schematically in Fig 5.

4. Assumptions:
As the process involves both fluid dynamics and heat transfer, some assumptions are made to simplify the model; they are listed as follows:

1-Melt in the domain is viscous and flow is laminar.
2-Contact resistance at the interface of melt- puddle and the roller surface is neglected by assuming perfect thermal contact.
3-Wheel acts as a perfect heat sink and wheel is filled with water to dissipate heat with heat transfer coefficient of inner wheel surface 22987.6 w/m².k
4. No slip exists between the wheel and melt and also between the melt and nozzle walls. Wheel surface is smooth with no resistance at melt-wheel contact.

5. No heat flux between the nozzle walls and melt (adiabatic). Radiation is neglected from the free surface of the melt.

6. Since amorphous ribbons are produced during PFMS process, the evolution of latent heat can be neglected. All physical properties of melt like density, specific heat, thermal conductivity are constant and independent of temperature except viscosity.

5. Based on these assumptions the governing equations can be written as:

Continuity equation:
\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0
\]

Momentum equation:
The Navier-Stokes equations can be derived by considering the dynamic equilibrium of a fluid element. They state that the inertial forces acting on a fluid element are balanced by the surface and body forces
\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial \left( \rho u_i u_j \right)}{\partial x_j} = \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho \frac{\partial \phi}{\partial x_i}
\]

Energy equation for the melt and surrounding air:
\[
\frac{\partial \left( \rho c_p u_i T \right)}{\partial t} + \frac{\partial \left( \rho u_i c_p u_j \right)}{\partial x_j} = \frac{\partial \left( k \frac{\partial T}{\partial x_j} \right)}{\partial x_j}
\]

Energy equation for the rotating copper roller:
\[
\frac{\partial \left( \rho \omega c_p u_l T \right)}{\partial t} + \frac{\partial \left( \rho \omega c_p u_l u_j \right)}{\partial x_j} = \frac{\partial \left( k \omega \frac{\partial T}{\partial x_j} \right)}{\partial x_j}
\]

Two-phase flow (VOF method):
To represent the free surface flow of the molten metal in the air domain fractional Volume of Fluid (VOF) method is used. VOF method developed by Nicholas [21] in his work is the best suited interface tracking method currently in use. A large number of applications have been reported for incompressible as well as compressible flows. In this method, a scalar function \( F \) is introduced that satisfies the following conservation volume-fraction equation:
\[
\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0
\]

where the value of \( F \) defines the phase state of the control volume in the computational mesh:

\( F = 0 \) control volume is filled only with air phase

\( F = 1 \) control volume is filled only with liquid or solid phase

\( 0 < F < 1 \) at the air/liquid or air/solid interface

The thermo physical properties appearing in the transport equations are determined by the volume fraction presented in each control volume:
\[
\rho = \rho_p F + \rho_m (1 - F)
\]
\[
\mu = \mu_p F + \mu_m (1 - F)
\]
\[
C_p = C_{p,p} F + C_{p,m} (1 - F)
\]
\[
k = k_p F + k_m (1 - F)
\]

6. Boundary conditions:

**Nozzle Inlet:**
\[
U = 0, \quad V = v_{in} , \quad T = T_{in}, \quad F = 1
\]

**Crucible walls:** The crucible wall is adiabatic with no-slip boundary condition
\[
U = 0, \quad V = 0, \quad \frac{\partial T}{\partial y} = 0
\]

**Air left and Air top:** Pressure inlet boundary Condition.
\[
P = P_{atm}, \quad T = T_{atm}
\]

**Outlet:** Pressure outlet boundary condition:
\[
P = P_{atm}, \quad T = T_{atm}
\]

**Roller:** Moving boundary, \( u = 100 \text{ rad} \)

Outer Wall (Air Convective heat transfer boundary condition) Inner wall (Water convective heat transfer boundary condition)

![Fig 6. Boundary conditions](image-url)
7. Operation condition
The operation condition is considered as the standard room condition where the temperature is 288.16 k and the absolute pressure is equal to atmospheric pressure is 101325 pa and the gravitational acceleration is -9.81 m/s².

IV. TEMPERATURE DEPENDENT VISCOSITY:
The viscosity of the melt as a function of temperature is used to consider the phase transformation of the amorphous alloy. We assume it to be of the Vogel–Fulcher form commonly used to describe the viscosity variation of amorphous materials through the glass transition:

\[ \mu_{\text{eff}} = \mu_0 \exp \left( \frac{A}{T - C} \right) \]

A and C are material-specific constants. The viscosity of the alloy Fe Si B used in the model as a function of the temperature:

\[ \mu_{\text{eff}} = 0.10 \times \exp \left( -3.6258 + \frac{734.1}{T - 674} \right) \]

And for alloy Ni B:

\[ \mu_{\text{eff}} = 0.000166 \times \exp (2180/ (\text{temp} – 722)) \]

User defined function (UDF) is developed to consider the variation of viscosity with temperature.

V. SOLUTION METHODS:
Fluent use for multi-phase flow the control volume technique to convert the governing equation to algebraic equation that can be solved numerically. 2D space planar and pressure based controller solved with first order explicit unsteady formulation is selected to solve the fluid flow and heat transfer equations in the air domain and solid domain. The energy equation is activated and used to analyses the thermal energy and heat transfer within the computational domains. SIMPLE semi implicit method for pressure linked equation finite volume algorithm is used to solving Navier stoke equation to obtain the velocity distribution and pressure field. An explicit time marching scheme is used to solve VOF equation. Interfacial heat transfer between the puddle and the roller is included by considering coupled wall type of interfaces boundary.

The gravity acceleration is used in negative y direction and its value is -9.81 m/s². For good and accurate analysis having stability criterion and avoiding divergence to take place the courant number (the ratio of time step size in the calculation to the characteristic time transient of fluid element across a control volume ) is specified as 0.5, therefore the time step size is limited to the order of 10⁻⁶.

VI. MATERIAL PROPERTIES, GEOMETRICAL AND PROCESS PARAMETERS:
The molten metal alloys used in the present work are Fe₇₅-Si₂₅-B₁₃ and Ni B. The material of the roller is copper. Geometrical and process parameters used for theoretical and Computational approach are listed in Table 1.

<table>
<thead>
<tr>
<th>S No</th>
<th>Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Roller Radius, R (m)</td>
<td>0.3</td>
</tr>
<tr>
<td>2.</td>
<td>Roller rotation speed, w [rad/s]</td>
<td>100</td>
</tr>
<tr>
<td>3.</td>
<td>Slit width of nozzle, s (m)</td>
<td>0.0006</td>
</tr>
<tr>
<td>4.</td>
<td>Nozzle Wheel gap distance, d (m)</td>
<td>0.0003</td>
</tr>
<tr>
<td>5.</td>
<td>Crucible wall thickness, R_e (m)</td>
<td>0.004</td>
</tr>
<tr>
<td>6.</td>
<td>Ejection velocity of molten metal alloy, vₑ (m/s)</td>
<td>1.6</td>
</tr>
<tr>
<td>7.</td>
<td>Inlet Ejection temperature of molten metal alloy, Tₑ (K)</td>
<td>1535</td>
</tr>
<tr>
<td>8.</td>
<td>Water wall heat transfer coefficient, hₑ (W/m²K)</td>
<td>22987.8</td>
</tr>
<tr>
<td>9.</td>
<td>Air heat transfer coefficient, hₐ (W/m²K)</td>
<td>71</td>
</tr>
</tbody>
</table>

Table 1: Geometrical and Process Parameters

The thermo physical properties of the materials used for theoretical and computational approach are listed in Table 2.

<table>
<thead>
<tr>
<th>Materials</th>
<th>Density (kg/m³)</th>
<th>Specific Heat (J/kgK)</th>
<th>Thermal Conductivity (W/mK)</th>
<th>Viscosity (kg/m s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surrounding air</td>
<td>1.225</td>
<td>1006.43</td>
<td>0.042</td>
<td>1.7984E+05</td>
</tr>
<tr>
<td>Copper roller</td>
<td>7600</td>
<td>381</td>
<td>387.6</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 2: Air and Copper Properties

The thermo-physical properties of molten amorphous alloys Fe Si B and Ni B used in the model are listed in the table (3).

<table>
<thead>
<tr>
<th>Designation</th>
<th>Parameters</th>
<th>Ni B</th>
<th>Fe Si B</th>
</tr>
</thead>
<tbody>
<tr>
<td>ρ</td>
<td>Density</td>
<td>7870 kg/m³</td>
<td>7180 kg/m³</td>
</tr>
<tr>
<td>Cp</td>
<td>Specific heat</td>
<td>440 J/kgK</td>
<td>544 J/kgK</td>
</tr>
<tr>
<td>K</td>
<td>Thermal conductivity</td>
<td>90 W/mK</td>
<td>8.96 W/mK</td>
</tr>
<tr>
<td>μ</td>
<td>Viscosity</td>
<td>μ(T)</td>
<td>μ(T)</td>
</tr>
<tr>
<td>σ</td>
<td>Tension</td>
<td>1.7 N/m</td>
<td>1.2 N/m</td>
</tr>
</tbody>
</table>

Table 3 (3)
VIII. RESULTS

A. Appearance of Air pockets under the melt puddle:

Air pockets appear under the melt puddle as shown in (fig 7) due to the suction of ambient air as the melt comes in contact with the moving substrate created by a negative pressure behind the upstream meniscus. Thus the air pockets reduce the contact area on the moving substrate side surface of the ribbon and decrease the stability to form ribbon with irregularities. The high cooling rate of the molten alloy relies on a good contact between melt and substrate, which is determined by fluid pressure near the contact surface in the puddle.

Fig. (7) Appearance of air pockets beneath the melt puddle

Higher melt injection velocity results in smaller negative pressure region in the rear part of the melt puddle which can alleviate the occurrence of air pockets on the substrate side of the ribbon.

Ribbon surface irregularities and reductions are formed because of negative pressure gradient in the melt near the contact surface between puddle and the impinging air and ratio of these reductions are high at initial time periods and prevent ribbon to be formed continuously as shown in the figure 8.

B. Development of melt puddle at different time periods for two kinds of alloys at identical process parameters:

Fig. (8) Reductions and Irregularities

Fig (9) Difference in shapes of melt puddles with two different alloys.

Fig (10). Melt puddle of Fe Si B

Simulation results show that the melt puddle of the Fe-Si-B alloy stabilizes at 10 milliseconds as shown in figure (10) which is in agreement with previous work of Durga Prasad (1). The stability of the melt puddle with Ni-B alloy occurs earlier at a time of 3 milliseconds which is in agreement with the simulation results of Bussman et al.(15). This is attributed to the difference in thermo-physical properties of the two alloys such as: density and thermal conductivity. Additionally, the difference in the puddle shapes fig.(9) for the two alloy combinations is also partly due to the difference in the variation of viscosity with respect to temperature as in the Vogel-Fulcher equation.
C. Effect of Heat Conduction into the moving substrate:

Heat conduction between the molten metal and moving substrate causes the temperature to increase inside the roller. The temperature contours inside the drum after 10 milliseconds for both the alloys in the fig below shows that the heat penetration inside the moving substrate for Ni-B alloy is greater than for Fe-Si-B alloy which is probably due to the early stability of the melt puddle of Ni-B melt (approximately 3 milliseconds) and the good contact between the melt puddle and roller surface whereas the heat transfer in the case of Fe-Si-B is happening slowly, as shown in fig (11 a&b).

D. Ribbon thickness of (Fe-Si-B & Ni-B) amorphous alloys:

Thickness of Fe-Si-B = 45 micro meter

Thickness of Ni-B = 33 micro meter

Fig. (12) Ribbon thickness of amorphous alloys

As shown in the fig. 12. The thickness of amorphous alloys differs due to the different glass formation temperatures, different thermo physical properties like density and effect of interfacial heat transfer between two alloys.

E. Variation of roller surface temperature of amorphous alloys:

The variation of roller surface temperature along the roller surface for different cycles is shown in (Fig. 12 a&b) slightly changes between two cases. The steep rise in the roller temperature at 0.1 mm indicates that molten metal touches the roller surface at that point. As the number of cycles increases the surface temperature at the point where puddle touches the roller increases. With the increase in number of cycles the puddle length increases and the molten metal is concentrated near the upstream meniscus and as a result the point of steep rise in
temperature shifts to the left. Further along the length of the roller the temperature decreases and reaches 350K. The maximum heat transfer coefficient at the drum surface is $2 \times 10^8$ W/m$^2$K. In real-time situation there will not be a sudden drop in the surface temperature as the water circulating will not take away the entire heat from the roller surface. Hence, to include the complete physics of the problem, interfacial heat transfer between the melt puddle and the roller surface is considered by employing conjugate (liquid/solid) heat transfer boundary condition.

![Fig (12 a) Roller surface temp of Fe Si B](image)

![Fig (12 b) Roller surface temp of Ni B](image)

**F. Streamlines and velocity vector:**

Streamlines and velocity distribution of the melt puddle and the surrounding air at different cases are plotted to explain the fluid flow, as shown in Fig. 13 (a) & (b). Recirculation zones with zero velocity forms near the nozzle wall on both sides of the melt puddle. The direction of the recirculation zones in the downstream meniscus is contrary to the direction of the recirculation zones in the upstream meniscus. At the surface of roller wall the velocity of the melt at the reaches the velocity of the roller due to the viscosity.

**VIII. CONCLUSION**

1- Numerical simulation based on the assumption of inconstant wall temperature boundary condition is able to study the melt puddle development with time and temperature distribution in the drum.

2- The melt puddle shape is different between alloys because the effect of in constant viscosity which is function of temperature and also surface tension.

3- Stable melt puddle is formed in the nozzle-wheel gap after 10 ms for Fe Si B and after 3 ms for Ni B and continuous ribbons of amorphous alloy appear after stabilization of melt puddle.

4- The thickness of amorphous alloys differs due to the different glass formation temperatures, different thermo physical properties like density and effect of interfacial heat transfer between two alloys.

5- Under the process parameters simulated, the pressure behind the upstream meniscus is slightly below
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atmospheric pressure, which facilitates air ingress between the melt puddle and moving substrate causing an unstable melt leads to formation of irregular amorphous trips. This can be overcome by increasing injection velocity and decreasing nozzle-moving substrate gap.

6-The heat penetration inside the moving substrate for Ni-B alloy is greater than for Fe-Si-B alloy which is probably due to the early stability of the melt puddle of Ni-B and the good contact between the melt puddle and roller surface whereas the heat transfer in the case of Fe-Si-B is happening slowly.

IX. REFERENCES

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