CFD Modeling and Simulation in Materials Processing
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Computational Fluid Dynamics (CFD) is a sophisticated method that uses mathematical equations and computer algorithms to simulate fluid flow, heat and mass transfer, and other related phenomena in a defined system. CFD modeling and simulation tools can successfully be tailored to capture multiscale and multiphase phenomena in complex material processing systems. Recently, CFD modeling and simulation technology has grown significantly in the manufacturing sector as often being the only efficient way to design, analyze and optimize complex manufacturing processes. We anticipate that more CFD tools will be implemented in the near future by industries related to materials processing to solve complex multiscale and multiphase engineering problems.

This book contains the proceedings of the symposium “CFD Modeling and Simulation in Materials Processing,” which was held during the TMS Annual Meeting and Exhibition, Orlando, FL, March 11-15, 2012. The objective of this symposium was to bring together experienced scientists and engineers that are involved in the modeling of multiscale and multiphase phenomena in material processing systems.

The symposium focused on the CFD modeling and simulation of metal processes including controlled melting and solidification processes such as EMS (electromagnetic stirring), UST (ultrasonic technology), and mold (mechanical) vibration, steelmaking processes, processes related to extractive metallurgy, advanced casting technologies (including refining of metals, foundry near-net-shape casting (such as investment casting and printing mold technologies), semisolid metal casting, ingot/roll casting, centrifugal casting, continuous casting), friction stir welding, heat treating (including water quenching), remelting (VAR/ESR/PAM/EBM) processes; multiscale modeling of PEM fuel cell systems, modeling of SOM electrolysis and recycling of Magnesium, CFD modeling of the carbothermic Aluminum process, environmental modeling (e.g., fuming during metal refining) and surface engineering processes (such as induction and scanning laser epitaxy processing). The symposium also dealt with applications of CFD to engineering processes and demonstrated how CFD can help scientists and engineers to better understand the fundamentals of engineering processes.

We expect that the papers collected in this book and ensuing discussions at the conference will continue to advance our understanding of various multiscale/multiphase/multicomponent phenomena occurring in materials processing systems and further promote the application of CFD models to solve complex engineering problems.

Finally, the editors of this book would like to acknowledge the efforts of all the contributors. Special thanks are due to Chris Wood and Matt Baker from TMS who supported our efforts of developing this symposium and helped us process all of the papers published in this book.

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Adrian S. Sabau received an Inginer Diplomat of Mechanical and Materials Processing degree from the University of Craiova, Romania and PhD degree in Mechanical Engineering from Southern Methodist University in 1996. In 1999, Dr. Sabau joined Oak Ridge National Laboratory as a Research Staff Member of the Materials Science and Technology, where he currently is a Senior Research Staff Member since 2008. Dr. Sabau is the recipient of two R&D 100 awards in process sciences. Dr. Sabau seeks to advance the materials processing, metal casting, photonic processing, and materials for energy applications through the development of computational and experimental methodologies for the property measurement, process analysis, and materials behavior in response to conditions experienced in service, such as oxide exfoliation in steam boiler tubes. The algorithm for microporosity prediction during casting solidification was implemented in the commercial casting software ProCAST. Dr. Sabau published more than 108 technical papers.

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CFD Modeling and Simulation in Materials Processing

CFD Modeling in Materials Processing I

Session Chairs:
Lifeng Zhang
Raj Venturumilli
FLUID FLOW, SOLIDIFICATION AND INCLUSION ENTRAPMENT DURING STEEL CENTRIFUGAL CASTING PROCESS

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Keywords: Centrifugal Casting, Steel, Fluid Flow, Inclusions, Entrapment

Abstract

The current study investigated the multiphase fluid flow, heat transfer, solidification of the steel, and the motion and entrapment of inclusions during the centrifugal casting process using FLUENT software. User-defined functions (UDFs) were developed to add velocity with a value related to the rotation speed and radial distance to the solidified steel, to exert a centrifugal force to the motion of inclusions, and to add the entrapment condition of inclusions at the solidifying shell and export the entrapment locations of the inclusion. The calculation shows that there are two peaks of inclusions along the thickness of the produced tube: one at close to outer surface and another one close to the inner surface of the tube. With a larger rotation speed, inclusions tend to be entrapped more towards the inner surface. The calculation agrees well with the industrial measurements.

Introduction

Centrifugal casting is used to produce cylindrical or hollow products, such as tanks, pipes and poles. It is both gravity and pressure independent. For round billet casting, molten steel is poured into an open-ended, water-cooled mold. Via rotation, the centrifugal force is in effect “liquid forging” or pressure casting so that molten metal is forced against the mold wall under relatively high pressure. The centrifugal force along with the rapid cooling effect of the chilled mold induces directional solidification across the casting wall under forced feeding conditions. Horizontal centrifugal casting involves pouring molten metal into a cylindrical mold spinning around its axis of symmetry, as shown in Figure 1. The casting mold keeps rotating with a speed of 300-3000 rpm, which results in an acceleration of 100 times gravity within the liquid metal layer [1]. Defects in conventional static casting (such as sand casting) like internal shrinkage, gas porosity and nonmetallic inclusions are less likely to occur in horizontal centrifugal casting. It has been reported that the process improved the density of cast metal and increased the actual mechanical properties of the casting by 10-15% while providing a uniform metallurgical structure [2]. For horizontal centrifugal casting, the technological parameters influencing final product properties involve mold rotation speed (n), casting temperature (T), casting speed (V),
chemical composition and casting dimension. The rotation speed has the highest influence on the formation of microstructure and the quality of casting. Different studies have been carried out to investigate the distribution of inclusions in steel pipes produced by the centrifugal casting process. It was reported that the content and distribution of the nonmetallic inclusions in the centrifugal casting steel depended to a significant degree on the metal being formed and the field of the centrifugal force during solidification. Compared to the distribution of inclusions in the radial direction, segregation in axial direction is minor. The current authors have found inclusions at the fracture surface of the centrifugally cast steel product. Figure 2 shows an example of Al₂O₃-MnS inclusions at the fracture surface.

In addition to direct observations of steel samples of centrifugally cast products, there are other alternatives to investigate this complex phenomenon and provide more information on the operation of the casting process. Martinez et al investigated the stirring phenomena in horizontal centrifugal casting using water modeling. To determine the size of recirculation eddies, dusts were used as tracers that floated on the free surface and gathered along lines where fluid velocity was directed towards the external radial direction.

The current publication presents the fluid flow simulation and inclusion entrapment during the casting and solidification of horizontal centrifugally cast steel. Computational Fluid Dynamics (CFD) simulation was used. Several factors, such as flow pattern, rotation speed, temperature variation, and top surface profile, are discussed in order to evaluate the important operating parameters and enhance product quality.

**Mathematical Formulation**

**Turbulent Flow Model**

To simulate the motion of inclusions in a turbulent field, it is necessary first to calculate the turbulent fluid flow. This work modeled three-dimensional single-phase steady turbulent fluid flow in the horizontal centrifugally cast mold using the continuity equation and the Navier-Stokes equations in a standard two-equation turbulence model.

The continuity equation was

\[
\frac{\partial (\rho u_j)}{\partial x_j} = 0
\]  

(1)
where \( \rho \) is density in kg/m\(^3\), \( u_j \) is a velocity component in the \( x_j \) direction in m/s. The momentum equation was

\[
\rho \frac{\partial (u_j u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \mu_{eff} \frac{\partial u_j}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \mu_{eff} \frac{\partial u_j}{\partial x_j} \right) + \rho g + F.
\]

(2)

where \( p \) is pressure in Pascal, \( F \) is a momentum source/sink term in N, and \( \mu_{eff} \) is the turbulence-adjusted effective viscosity in kg/m. The latter is calculated by

\[
\mu_{eff} = \mu_\ell + \mu_t
\]

(3)

where \( \mu_\ell \) is laminar fluid viscosity in kg/m\( \cdot \)s, and \( \mu_t \) is turbulent fluid viscosity in kg/m\( \cdot \)s. The standard k-\( \varepsilon \) two-equation turbulence model was used to determine the effective viscosity \( \mu_{eff} \).

Volume of fluid (VOF) multiphase model was employed to track the interface between the molten steel and the air. The VOF multiphase model was used to track the free surface moving through the computational grid by simultaneously solving another parameter, the volume fluid per unit volume, \( f_i \). It requires the converging of an additional conservation equation (Eq.(4))

\[
\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_j} \left( f_i u_j \right) = 0
\]

(4)

The following energy conservation equation was used to calculate the heat transfer in a casting mold,

\[
\frac{\partial}{\partial t} (\rho H) + \frac{\partial}{\partial x_j} (\rho u_j H) = \frac{\partial}{\partial x_j} \left( k_{eff} \right) \frac{\partial T}{\partial x_j} + Q
\]

(5)

where \( H \) is enthalpy or heat content in J/kg, \( k_{eff} \) is temperature-dependent effective thermal conductivity in W/m-K, \( T \) is the temperature field in K, and \( Q \) contains heat sources in W/m\(^3\).

Solidification Front Growth Model

Mushy zone is a zone in a solidifying alloy in which solid and liquid coexist. The growth of dendrites in this region can be modeled by several numerical models, such as the phase-field model, the cellular automaton model, and stochastic models, including the Monte Carlo Model. In the current study, the method of enthalpy-porosity \(^{101}\) is used. For this method, instead of tracking the accurate liquid-solid front, it treats the liquid-solid mushy zone as a porous zone. Furthermore, it uses the liquid fraction (0.0 - 1.0) to describe the mushy zone. When the material is in a liquid state, the liquid fraction is 1.0; when it has fully solidified, the liquid fraction becomes 0. The liquid fraction, \( \beta \), is defined as follows

\[
\beta = 0 \quad \text{if} \quad T < T_{\text{solidus}}
\]

(6)

\[
\beta = 1 \quad \text{if} \quad T > T_{\text{liquidus}}
\]

(7)

\[
\beta = \frac{T - T_{\text{solidus}}}{T_{\text{liquidus}} - T_{\text{solidus}}} \quad \text{if} \quad T_{\text{solidus}} < T < T_{\text{liquidus}}
\]

(8)

The heat transfer equation is the same as Eq.(5), while

\[
H = h_{ref} + \int_{T_{ref}}^{T} C_p dT + \beta L
\]

(9)

where \( h_{ref} \) is the reference sensible enthalpy, \( L \) is the latent heat, \( T_{ref} \) is the reference temperature.
The mushy zone is treated as a porous medium. To consider the momentum loss in this region when liquid phase becomes solid phase, the loss is represented by adding a sink term to the end of the momentum equation. The momentum sink and the turbulent sink term can be described as

\[ S = \frac{(1-\beta)^2}{(\beta^2 + 0.001)} A_{mush} \cdot \phi \]  

(10)

where \( A_{mush} \) is the mushy zone constant, and \( \phi \) is the variables such as the velocity and the turbulence quantity.

A UDF subroutine was developed, by which once the liquid fraction is less than a certain value, for example, 0.3, then steel will be imposed a fixed x-velocity and y-velocity from the rotation speed as Eqs.(12) and (13) respectively. The z-velocity will be as it is.

\[ V_x = -r \sigma \sin \alpha = -y \left( \frac{2\pi}{60} \right) \]  

(11)

\[ V_y = r \sigma \cos \alpha = x \left( \frac{2\pi}{60} \right) \]  

(12)

Inclusion Motion and Entrapment Model

Particles were modeled using both Eulerian and Lagrangian approaches. The Eulerian approach considers particles a continuous phase, whereas the Lagrangian approach treats particles as a discrete phase. Due to the low volume fraction of particles, the Lagrangian approach is always used to calculate the trajectory of particles by considering the force balance acting on them

\[ \frac{du_i}{dt} = \frac{18 \mu}{\rho_i d_p^2} C_D \left( u_i - u_p \right) + \frac{\rho_i - \rho}{\rho} g_i + \frac{1}{2 \rho_i d_p} \left( u_i - u_p \right) + \frac{\rho_i}{\rho} \frac{\partial p}{\partial x_i} \]  

(13)

where \( u_p \) is particle velocity at direction \( i \) in m/s, \( t \) is time in seconds, \( C_D \) is a dimensionless drag coefficient, \( Re_p \) is a particle Reynolds number, \( d_p \) is particle diameter in m, \( \rho \) is inclusion density in kg/cm\(^3\). The first term here is the drag force per unit of particle mass, the second term is gravitational force, the third term is the virtual mass force accelerating the fluid surrounding the particle, and the fourth term is the force stemming from the pressure gradient in the fluid.

To incorporate the stochastic effect of turbulent fluctuations on particle motion, the random walk model was used. In this model, particle velocity fluctuations are based on a Gaussian-distributed random number chosen according to the kinetic energy of the local turbulence. The random number is changed, to produce a new instantaneous velocity fluctuation at a frequency equal to the characteristic lifetime of the eddy. The instantaneous fluid velocity is then given by

\[ u = \bar{u} + u' \]  

(14)

\[ u' = \xi \sqrt{u'^2} = \xi \sqrt{2k/3} \]  

(15)

where \( \bar{u} \) is the mean fluid phase velocity in m/s, \( u' \) is random velocity fluctuation in m/s; \( \xi \) is a random number and \( k \) is the local level of turbulent kinetic energy in m\(^2\)/s\(^2\).

As boundary conditions for the particle motion, particles were assumed to be entrapped when the temperature of the steel where the inclusion was located was below 1775 K, corresponding to a liquid fraction of 0.3, as shown in Figure 3. This entrapment was controlled by a UDF.
programmed by the authors. The entrapment locations of inclusions were exported to a separate file using the author developed UDF.

Liquid Fraction = 0.3 = 0.6

Figure 3. Solidification fraction and inclusion entrapment

Calculation Parameters and Boundary Conditions

In the current study, the mold is 16 meters long and diameter is 0.288 m. Dimensions, parameters and boundary conditions are listed in Table 1. During an iteration, convergence is assumed to be reached if all the normalized un-scaled residuals \[ \| \] are smaller than \( 10^{-6} \). The mesh used is shown in Figure 4. In order to reduce the computation time, and improve computation quality, the mesh should be controlled to a reasonable number. In the current study, the entire domain contains 663,680 cells. FLUENT was used for the computation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mold length</td>
<td>16 m</td>
<td>Viscosity of liquid steel</td>
<td>0.0067 kg/m·s</td>
</tr>
<tr>
<td>Mold radius</td>
<td>0.212 m</td>
<td>Density of liquid steel</td>
<td>7020 kg/m³</td>
</tr>
<tr>
<td>Mold inlet radius</td>
<td>6 cm</td>
<td>Thermal expansion coefficient</td>
<td>( 1 \times 10^{-4} ) 1/K</td>
</tr>
<tr>
<td>Rotation speed</td>
<td>1000 rpm</td>
<td>Density of inclusion</td>
<td>5000 kg/m³</td>
</tr>
<tr>
<td>Inlet velocity</td>
<td>1.915 m/min</td>
<td>Latent heat</td>
<td>270000 J/kg</td>
</tr>
<tr>
<td>Turbulent energy</td>
<td>0.00001</td>
<td>Initial temperature</td>
<td>1853 K</td>
</tr>
<tr>
<td>Dissipation rate</td>
<td>0.00001</td>
<td>Liquidus temperature</td>
<td>1803.15 K</td>
</tr>
<tr>
<td>Pouring time</td>
<td>8.5 s</td>
<td>Solidus temperature</td>
<td>1763.15 K</td>
</tr>
<tr>
<td>Latent heat</td>
<td>270000 J/kg</td>
<td>Thermal conductive</td>
<td>34 W/m·K</td>
</tr>
<tr>
<td>Mold rotation speed</td>
<td>500-1000 rpm</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The filling process lasted 8.5 seconds. After the filling process, fluid flow (3D-VOF multiphase), heat transfer and solidification were considered. The initial temperature of the liquid phase was 1853K, and temperature of the air phase inside the mold was assumed to be 1400K. For the heat transfer boundary condition at the mold wall, the wall boundary condition was either fixed at 1400K or a mixed heat transfer condition was assumed including the effect of conduction, convection and radiation from the wall with a 1000 W/m²-K heat transfer coefficient, a 12 W/m-K thermal conductivity of the wall material, a 323 K free steam temperature and 0.7 external emissivity.

For the motion of particles, the density of inclusions was assumed to be 5000 kg/m³. Around 50,000 inclusions of each size were initially randomly distributed in the liquid phase after filling and allowed to move with the motion of the liquid steel.

Three Dimensional Simulation Results

Distribution of Centrifugal Force

The centrifugal forces are created by the circumferential motion. The linear velocity of a point on a rotating rigid object at a distance from the axis of rotation represents the tangential velocity of that point. For rotation about a fixed pivot point, the path of any point on a revolving body is a circle, and its linear velocity at any moment is always tangent to that circle. Therefore, the centrifugal force per unit volume can be defined as follows,

\[ f_c = \frac{\rho v^2}{r} \]  

where, \( f_c \) is the centrifugal force per unit volume, N/m³; \( \rho \) is the density of the mixture, kg/m³; \( v \) is the tangential velocity, m/s; and \( r \) is the radius from center to the point, m.

\[ r = \sqrt{x^2 + y^2} \]  

(17)

The centrifugal acceleration rate can be expressed by

\[ a_c = \frac{v^2}{r} \]  

(18)

The casting mold keeps rotating with a speed of 1000 rpm, which results in an acceleration of around 100 times gravity within the liquid metal layer. The distribution of centrifugal force is shown in Figure 5. The centrifugal force inside the liquid metal layer is much larger than other places in the pipe, which confines molten steel inside the thin layer and rotating with casting mold. From the Figure 5(b), we can see that the maximum centrifugal force on the mold wall is as large as \( 1.63 \times 10^7 \) N/m³; however in the center of the pipe the centrifugal force is close to 0 N/m³. Figure 6 shows the distribution of the centrifugal acceleration rate in the pipe. Since no density is involved here, the centrifugal acceleration rate decreases from the mold wall to the mold center, with a maximum value of 2320 m/s² at the mold wall.
Fluid Flow during Pouring and Rotation

In the current simulation, the ladle slide gate was assumed to be fully open resulting in a pouring time of 8.5 seconds. Figure 7 shows the pouring and rotating process during this period. At 0.3 s pouring, the molten steel touches the bottom of the tube mold. After that, the molten steel starts rotating with the tube, as shown in the Figure 7 (b). At 8.5 s, the molten steel covers the entire mold inner surface, and a liquid steel layer forms.
More detailed information is revealed by observing the interface between the air phase and the molten steel phase inside the mold, as shown in Figure 8. At the end of pouring, 8.5s, the interface between air and steel becomes rough. Metal droplets in air and air penetration into the molten steel are observed, which will induce serious reoxidation from the air and generate new oxide inclusions, especially near the middle length regions of the mold. The simulation shows that at 9.0 s, the interface is still rough implying air reoxidation. Therefore, more time is required to fully stabilize the air-steel interface during the rotating, cooling and solidification process.

Inclusion Motion during Filling

A simulation was done for the filling process together with injection of 50000 inclusions. In this simulation the heat transfer and solidification are not included. The time step is 0.0001 s. Four-
second filling was simulated together with the motion of these inclusions. The computation time is extremely large and could be up to 3 months to complete. The simulation results are shown in Figure 9. Inclusions are dispersed quickly with the filled steel.

![Figure 9. Inclusion motion during filling (Iso-surface of 0.9 fraction of steel, and inclusion locations)](image)

Figure 10 shows the interface between the steel phase and the air phase, the temperature on the interface, and inclusion entrapped locations (black dots) and motion locations at 10.90 s (2.40 s after the filling) with a fixed mold wall temperature as 1400 K. The interface was not flat, and fluctuated with time, and may tend towards a flat shape after a certain time, which will be
determined by future calculations. The black dots were the locations of entrapped inclusions, where the temperature of the steel reached the temperature 1775K, corresponding to a 0.3 liquid fraction. The green dots were the inclusions that still moved with the fluid flow. Some inclusions were entrapped close to the wall since the steel cooled there first. Certain amount of inclusions were also entrapped close the interface between the liquid steel and the air since the initial air phase was assumed to be 1400K.

Figure 10. The interface between the steel phase and the air phase, the temperature on the interface, and inclusion entrapped locations (black dots) and motion locations (green dots) at 10.90 s (0.90s after the filling) with a fixed mold wall temperature as 1400 K.

Figure 11 shows the position of inclusions changing with time, indicating that inclusion moved around with rotation of the domain and more and more inclusions were entrapped with time increasing. Figure 11b indicates that inclusions were always in the steel phase since our centrifugal force UDF reveals that once inclusions enter the air, the centrifugal force direction is outwards and thus inclusions move back to the steel phase.

Figure 11. The locations of entrapped inclusions (black dots) and moving inclusions (green dots) in the domain with a fixed mold wall temperature as 1400 K.