Development of a New Simulation Method of Mold Filling and Solidification Based on the SIMPLER Algorithm

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A new combined method is to be introduced and applied to the mold filling and solidification process. In the present method, the SIMPLER algorithm was adopted to solve the momentum and energy equations. The VOF (Volume of Fluid) method was also adopted to track the free surfaces in the filling process and the Equivalent Specific Heat Method to solve the phase change heat transfer problem in the solidification process. The staggered grid system was used to prevent the false velocity field and the non-uniform control volumes were used to improve the efficiency of calculation. The standard DAFA (donor and acceptor flux approximation) method was adopted in the VOF method. In order to verify the new combined method, the numerical results were compared with the experimental results of mold filling and other simulation methods. It is concluded that the new method can be used as an effective simulation method for the simulation of mold filling and solidification in the casting processes.

KEY WORDS: combined algorithm; mold filling; solidification; SIMPLER algorithm; VOF method; Equivalent Specific Heat method; numerical simulation; normal stress condition; tangential stress condition; resistance circuit.

1. Introduction

During the last decade, numerical studies on the casting processes have actively been done to develop numerical models for casting processes. As a result, a number of studies have been reported on the applications of mold filling or solidification in the casting processes. The conventional mold filling models are mostly based on the explicit scheme and their solution algorithms are SMAC or SOLA, while the most solidification models are based in the implicit scheme. If the filling process is only considered, the implicit scheme does not have much benefit since it needs more time to finish the calculation than the explicit scheme when the same time steps are applied. But the casting processes do not consist only of filling but also of solidification. And due to the latent heat release, it takes more time for solidification than for filling physically. If the explicit time steps are applied even during the solidification, it will take too long time to finish the simulation. That’s one of the reasons why lots of researches on solidification (without the filling process) are adopting the SIMPLE algorithm. Recently, Hong et al. suggested the solution for the mold filling in the curved-shaped and thin-walled castings based on the Body Fitted Coordinate system. The FEM may also be a useful method to model numerically a curved shaped cavity because it uses triangular elements as well as rectangular ones. However, the BFC (Body Fitted Coordinate system) method needs larger computational time even in a simple shaped cast, and it is a very complicated process to model a mold and cast at the same time. The FEM has been known to be less suitable to predict the incompressible flow, and also to be much less effective in terms of the computational time and memory size than those methods based on the FDM (Finite Difference method) or FVM (Finite Volume method). So both the BFC scheme and the FEM method are unsuitable to be applied to the general casting processes.

In the present study, a new combined method (SIMPLER-VOF with Phase Change) was developed to simulate not only the mold filling process but also the heat transfer phenomena both in a cast and in a mold. Though the Line By Line (LBL) method based on TDMA (Tri-Diagonal Matrix Algorithm) is the conventional method for most implicit schemes, the Point By Point (PBP) method has been adopted to avoid including flow calculations in a mold and empty zone. But the PBP method is used only for the flow field calculation during filling. In order to verify the new method, the experimental results for phase change heat transfer of ours and mold filling of other’s were referred to.

2. Computational Method

2.1. Basic Equations

The casting processes include several complicated physical phenomena. Like other Computational Fluid Dynamics
problems, the continuity equation, the momentum equation and the energy equation are the partial differential equations that are essential in the numerical analysis of the casting process. In addition, molten metal is to be filled into an empty confined region from an inlet or inlets. The phase change interface also moves as the cooling proceeds. Thus the volume fraction equation is also to be solved together with the momentum equation, and the unsteady solidification phenomenon is to be treated as a source term in the energy equation. The aforementioned partial differential equations that describe the transport phenomena can be represented in a generalized form Ref. 17) as Eq. (1). This equation contains four terms. They are, from left to right, the unsteady term, the convection term, the diffusion term, and the source (or sink) term. Individual equations can be recovered from Eq. (1) by assigning specific meanings to the superscripts and subscripts in the Cartesian Coordinate system.17) The coefficients are determined by the intensity of diffusion and convection, and the subscripts (r) and (s) represent the directions of flow.

\[
\frac{\partial}{\partial t} (\rho \Phi) + \frac{\partial}{\partial x_j} (\rho u_j \Phi) = \frac{\partial}{\partial x_j} \left( \Gamma_j \frac{\partial \Phi}{\partial x_j} \right) + S \quad \text{...............(1)}
\]

As a result, the final discretized equation is given by

\[
a_{ij} \Phi_{ij} = \sum_{n} a_{ij} \Phi_{ij} + b \quad \text{..................(2)}
\]

where \( a_{ij} \) is the flux coefficient, and \( b \) is the body forces, the unsteadiness etc.

The volume fraction transport equation is discretized in a different way because the VOF method is based on the explicit scheme, while the SIMPLER algorithm is a Semi-Implicit method.1, 17) So the discretized equation is given by

\[
\Phi^{n+1} = \Phi^n - \Delta \frac{\Delta t}{\Delta x_j} \left( u_j \Phi^n \right) \quad \text{...............(3)}
\]

where the superscripts \( n+1 \) and \( n \) mean the present and previous time stage value. According to the Donor and Acceptor Flux Approximation (DAFA),3) and the cell flux \( \Delta (u_j \Phi^n) \) is given as follows.

\[
\Delta (u_j \Phi^n) \Delta t = \text{sgn}(u_j^n) \min [\Phi_{ij}^n + \Delta t (CF, \Phi_{ij}^n)]
\]

\[
CF = \max ((F - F_{AD}) | u_j^n \Delta t |) \quad \text{...............(4)}
\]

\[
(F) = \max [F_{DM}, F_{DM}, 0, 0] \quad \text{...............(5)}
\]

The selection of the subscripts \( D, DM \) and \( AD \) is identical to the conventional DAA.1, 3)

Since the explicit scheme (VOF) and implicit scheme (SIMPLER) were combined together, the time steps are limited by the explicit scheme during filling. The time step is determined by:

\[
\Delta t < \text{MIN} \left[ \frac{\delta x_j}{u_{ij}, k}, \frac{\delta y_j}{v_{ij}, k}, \frac{\delta z_j}{w_{ij}, k} \right] \quad \text{...............(5)}
\]

This is to make sure that the volume fraction can not move through more than one cell in one time step, and it's applied only during the mold filling.

### Table 1. Definitions of \( \Phi, \Gamma, \) and \( S \) in Eq. (1).

| Equation                  | \( \Phi \) | \( \Gamma \) | \( S \) |
|--------------------------|----------|----------|----------|
| Continuity Equation      | \( \rho \) | \( \rho \) | \( \rho \) |
| Volume Fraction          | \( \rho \) | \( \rho \) | \( \rho \) |
| Momentum Equation (velocity) | \( u \) | \( \mu \) | \( -\rho \sigma_v \) |
| Energy Equation (temperature) | \( T \) | \( k \) | \( \rho \epsilon_{ij} (\Delta T) \) |

\( \mu \) : Dynamic viscosity, \( k \) : thermal conductivity, \( \epsilon_{ij} \) : specific heat, \( \rho \) : density, \( \Delta T \) : evolution of latent heat

![Fig. 1. Various boundaries in casting process. (a) Grid system with one example of free surface boundary. (b) Boundary between cast and mold.](image-url)

### 2.2 Boundary Conditions and Phase Change Heat Transfer

The no-slip wall boundary condition was applied at the mold walls, and the normal and the tangential stress conditions were applied on the free surfaces.3, 4) Specifically, the normal and the tangential stress conditions affect the accuracy of the free surface motion. The following equations have to be satisfied simultaneously on the free surfaces.

**Normal stress condition**

\[
P_{\text{free-surface}} = \delta_{ij} \sigma_{ij} + P_{\text{applied}}
\]

**Tangential stress condition**

\[
\tau_{ij} = 0 \quad (i \neq j) \quad \text{...............(7)}
\]

The basic idea of the SIMPLER algorithm is that the pressure gradient arouses the velocity. In light of this concept, since the normal stress condition that explains the pressure on the free surface as the equivalence of the stresses (expressed in terms of velocity vectors), the SIMPLER algorithm is also beneficial in treating the free surface problems. As one example, consider situation in Fig. 1(a).
To solve Eq. (8), the pressure \( p_s \) is needed and it can be attained using the normal stress condition. \( i=j=y \) is obtained in Fig. 1(a) and gives the following differential and discretized equations from Eq. (6) when \( p_{\text{applied}} = p_{\text{reference}} = 0 \):

\[
2\mu \frac{dv}{dy} = p_{\text{free-surface}} \Rightarrow p_{\text{free-surface}} = 2\mu \frac{v - v_t}{\Delta y_p} \quad (9)
\]

\( v_t \) can be determined using the volume of fluid in the cell \( P \) and the continuity equation, which is another practical way of using the VOF method. Again in Fig. 1(a), \( u_n \) is expressed as follows.

\[
a_n u_n = a_r u_r + a_w u_w + a_m u_m + b(p_m - p_f) A \quad \text{...............(10)}
\]

Now, we need to know \( u_w \) in order to make Eq. (10) fit with the equations for the filling process. As can be seen from Fig. 1(a), \( u_w \) is not the velocity in the fluid region. Though the symmetric boundary conditions on the free surface can be found in some researches especially when there isn’t a wavy free surface motion, \( 10,11 \) the tangential stress field as in the convectional Equivalent Specific Heat model isn’t a wavy free surface motion, \( 10,11 \) the tangential stress face can be found in some researches especially when there is no wavy free surface motion.

3. Results and Discussion

3.1. Validation of Phase Change Process

Validation for the filling process is mentioned in the next section with the experimental results of Mampaey’s.\(^{16}\)

For the phase change process, the experimental method was adopted, i.e., the cooling curves of mold and cast were gained through an experiment, and the simulation result was presented here to verify the numerical model for the new combined algorithm. The details of the experimental method was skipped here, but can be referred from the literature\(^{15} \) in detail. Figure 2(a) and Table 2 show the experimental model and properties of mold and cast, and Fig. 2(b) shows the cooling curves from 4 different locations comparing the experimental and numerical results. The Y-axis is the temperature and the X-axis is the elapsed time. The mold temperature (TC1, TC2) changes steeply in the early stage. The reason for slightly higher temperature in TC2 is the natural convection in molten metal: that is, the cooler liquid metal goes down and the hotter liquid metal goes up in the mold cavity. From the middle stage of solidification, the temperature varies slowly and finally keeps constant. It’s because the heat gain from the cast and the heat release to the outer air are balanced as solidification proceeds. The temperature variation curves of mold from numerical calculation showed good agreement with the experiment. The cast temperature (TC3, TC4) drops steeply from the start. But the slope of cooling curve becomes slow soon as the latent heat begins to be released.

The evolution of latent heat also makes the slope of cooling curve in the cast zone much slower than in the mold zone. The temperature variation curves of cast from numerical calculation also showed good agreement with the experiment.

3.2. Mold Filling Simulation and Comparison with Experimental Results and Other Simulation Schemes

The new SIMPLER-VOF method has been applied to simulate the mold filling problem, and was compared with the simulation and experimental results of other researchers.
reported in the journals. Xu and Mampaey\textsuperscript{16} et al. reported about their orthogonal-curvilinear-coordinate method which is based on the VOF scheme, employing a structured non-orthogonal mesh system. They proved their scheme to be an acceptable simulation tool by comparing the results of simulation with the experimental results made on the mold filling with a curved gating system. Their simulation and experimental models were adopted in the present study in order to verify the new numerical scheme. The results based on BFC\textsuperscript{12} were also shown together, which are known to be the most accurate numerical results so far. The dimensions of the physical model and the result of grid generation in the present study are shown in Fig. 3 and the material properties in Table 3. A non-uniform grid comprised of (96, 71, 31) control volumes was used. The mesh was finer near the boundaries and the fluid region, while it was coarser in the mold region. A total of 211,296 meshes were applied with various mesh sizes to concentrate more mesh cells in the region to be filled with molten metal than in the mold region. The mesh cells used in the present study have the minimum edge length of 0.1$\times$10$^{-2}$m and the maximum edge length of 1.5$\times$10$^{-2}$m. It took 7 h to finish the calculation of filling with Pentium III-800 MHz laptop.
when only the flow calculation was engaged. Though it took less time with the present method than with the numerical model based on the BFC (16 hr), this does not mean that the SIMPLE-BFC-VOF is useless approach for the mold filling, because the BFC system is known to be the more accurate and more effective simulation method than any other numerical model when a cast is curved and thin-walled.

Figure 4 indicates the filling sequences in the mold cavity through the curved gating system: (a) and (b) are the experimental and simulation results by Mampaey et al.\textsuperscript{16} (c) is the simulation results by the BFC calculation\textsuperscript{12} and (d) is the simulation results of the present SIMPLER-VOF method. As shown in Fig. 4(a), the experimental observation shows that the melt passing through a curved gate is ejected into the mold cavity with a slight slope against the vertical axis and it reaches up to the top plane of the mold cavity until the end of the filling. It is found in Fig. 4(c) and 4(d) that the simulations by the BFC and the new method can predict exactly the filling pattern and sequences for this model, while the simulation by Mampaey \textit{et al.} predicts that the molten melt enters into the mold cavity rather vertically, which is slightly different from the experimental observation. It can also be said that the present SIMPLER-VOF method predicts exactly the successive filling pattern in the curved-shape mold cavity as can be seen in the rest of the figures.

3.3. Solidification Process Simulation

While Mampaey \textit{et al.} did not experiment or simulate for the solidification process, the solidification sequence was simulated in the present study using the material properties (thermal conductivities of cast and mold, specific heats, Latent heat, Heat transfer coefficients at boundaries) found in the text\textsuperscript{19} and they are shown in Table 3. Fusion temperature was assumed to be 1 810 K with latent heat released uniformly in 1 785 K < T < 1 810 K, and molten metal was supplied at the temperature of 1 860 K. The initial mold temperature was assumed to be 373 K and ambient temperature 298 K. The figures in right hand side in Fig. 5 indicates the solidification sequences at the completion of the filling, at the 20% solidification fraction, and at the 60% solidification fraction. Though the elapsed time for the completion of the filling was just around 1.3 s, the temperature field in the cast region was neither uniform nor close to the initial temperature of the melt on the completion of the filling as can be seen in the first figure. This means that it is need to carefully consider the thermal properties of a melt and a mold as well as the working conditions when the assumption of a uniform temperature in a casting at the completion of filling due to the rapid filling process is made. While the solidification proceeded along the whole boundary in the left figure of the second figures, the final solidification occurred near the entrance to the cavity [the left figure of the last figures] due to the cooling capacity as well as the thermal inertia of the mold. The temperature of the mold became higher as the solidification proceeded. But the temperature variation was less steep than that in the casting region due to the thermal inertia (due to low thermal conductivity, high specific heat – -) of the sands. The figures in left hand side in Fig. 5 show the temperature distributions in a plane of mold adjacent to the cast. The heat loss from cast to mold can be calculated like follows.

![Fig. 4. Mold filling sequences in a mold cavity having a curved gating system. (a) Experimental results by Mampaey et al\textsuperscript{16}: 0.666, 0.803, and 1.001 s. (b) Simulation results by Mampaey et al\textsuperscript{16}: 0.603, 0.803, and 1.001 s. (c) Simulation results based on BFC\textsuperscript{12}: 0.6, 0.8, and 1.0 s. (d) Simulation results by the present SIMPLER-VOF method: 0.6, 0.8, and 1.0 s.](image-url)
Equation (14) means that the heat loss from cast to mold is affected by temperatures in mold and cast as well as their properties. It is observed in Fig. 5 that the mold temperature varies according to both location and elapsed time as the solidification proceeds in the cast. So the effects of mold concerning the heat transfer during filling and solidification are very important in the simulation of the casting processes as well as in real casting processes.

5. Conclusion

A new simulation method, based on the coupling of the SIMPLER algorithm, the VOF (Volume of Fluid) method, and the Equivalent Specific Heat method has been developed for the simulation of both mold filling and heat transfer in the casting processes. The present SIMPLER-VOF (with Phase Change) method was verified by comparing the simulation results with the experimental results reported in the journals. It can be concluded that the present SIMPLER-VOF method can be used as an effective numerical tool for the simulation of the casting processes. In addition, when applied to the thin-walled mold cavity with a curved gating system, the present SIMPLER-VOF method gave predictions not only for the free surface movement during filling but also for the phase front tracking during solidification including the heat transfer in the mold. In the case of the filling process, the prediction was as good as those based on the non-orthogonal mesh system and the BFC system.

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