A Semi-Lagrangian Method Based on MAC and Its Application in Fluid Simulation of Casting Filling Process

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Abstract

In this paper, a marker-and-cell based semi-Lagrangian method, which combines the advantages of Lagrangian and Eulerian perspective, is introduced to simulate the metal flow during casting filling process. This method treats fluid in terms of a vast collection of particles with some physical properties that move around, naturally bypass the unique complex free interface tracking problem in Eulerian perspective. For the interior of the fluid, the efficient Projection method is used to solve the incompressible Navier-Stokes equations. On the other hand, the diffusion equation is solved on the background grid by mapping the information carried by the particles to the grid, thus avoiding the inconvenience of field description in Lagrangian perspective. And the level set method is introduced to describe boundary. In order to study the application of this method in the casting field, two examples are given with this method and the widely used VOF method. The results show that this method can produce sharp and discontinuous fluid interfaces, which is closer to the casting process with high filling speed.

Keywords: marker-and-cell, semi-Lagrangian method, casting filling process, fluid simulation

Introduction

In the field of casting, computational fluid dynamics is mainly used to simulate the metal filling process and analyze defects that may occur during the filling process, such as cold shut[1] and oxide inclusion[2]. The flow front of the molten metal plays a very important role in analyzing the filling defects. The mainstream free surface tracking methods in casting simulations use a fixed grid. Methods like VOF (Volume-of-Fluid) [3], Level set[4], and CLSVOF (Coupled Level Set and Volume-of-Fluid)[5] are widely used. This kind of methods uses continuous functions to indicate the free surface, in a pure Eulerian perspective. Traditionally, the main difficulty in using these methods has been the maintenance of a sharp boundary[6]. Methods that use separate, boundary-fitted grids for each phase[7-9] may offer potentially the highest accuracy, are rarely used in casting simulations because of their complexity.

Another class of methods is the particle-based “meshfree” methods, such as MPS (Moving Particles Semi-implicit)[10], SPH (Smoothed Particle Hydrodynamics)[11], DPD (Dissipative Particle Dynamics)[12,13]. The absence of a mesh allows Lagrangian simulations, in which the particles can move according to their own state. However, when calculating the force of particles, we have to find the location of neighboring particles. To avoid being n-body problems, some complex data structures such as the multi-grid technique should be applied. Besides, a casting is usually very complex in geometry that requires many particles. The relatively low computing efficiency makes them very difficult to be applied to casting simulation.

The MAC (marker-and-cell) method[14] is a semi-lagrangian method that between the fixed grid and mesh-free methods. It uses a fixed grid to describe the interior of the fluid, and marker particles to indicate fluid configuration. With a structured grid used, it not only has the advantage of fixed grids in solving NS equations but also has the advantage of mesh-free methods in advancing fluid front. However, it is rarely used in casting simulations although it is very popular in the field of computational fluid dynamics. In this paper, the MAC method, coupled with the level set approach to describe the complex boundary, is introduced to simulate the casting filling process. Through the actual calculation case, the potential applications and limitations of this method in the casting filling simulation process are discussed.

Description of the Method

Outline of procedure

The governing equations for viscous incompressible flows are the continuity and the Navier-Stokes equations as follows[15]:

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

and

$$\frac{D\vec{u}}{Dt} = -\nabla\varphi + \nu\Delta\vec{u} + \vec{f} \tag{2}$$

Where $\varphi = P/\rho$ is the ratio of pressure to density, it is usually referred to as "pressure" simply, and the triangular symbol Δ represents the Laplacian. Using the efficient Projection procedure[16], a Poisson equation for pressure can be obtained:

$$\Delta\varphi^{n+1} = \frac{\nabla \cdot \vec{u}^*}{\delta t} \tag{3}$$

$$\vec{u}^* = \vec{u}^n + \delta t\left(\nu\Delta\vec{u}^n + \vec{f}^n - \vec{u}^n \cdot \nabla\vec{u}^n\right) \tag{4}$$

The superscript "n" and "n+1" denotes the cycle number, for example, φ^{n+1} is the pressure value of cycle n+1. Solving Eq.(3) and substitute the pressure back to Eq. (2), then the velocity field of cycle n+1 is obtained:

$$\vec{u}^{n+1} = \vec{u}^* - \delta t \cdot \nabla\varphi^{n+1} \tag{5}$$

The overall procedure is based on the classical Marker-and-Cell method developed by Harlow and Welch [14]. For a calculation cycle, there are six steps as follow:

(1) Compute pressure. Solve the Poisson equation of pressure based on the velocity and liquid level set field.

(2) Update velocity. Update the velocity field by substituting back the new pressure field to the Navier-Stokes equation.

(3) Convection. The marker particles are moved according to the velocity components in their vicinities, with temperature interpolated from background cells. Adjustments are made when particles across cell boundaries.

(4) Tracking the free surface. Update the liquid level set value according to the positions of the marker particles.

(5) Compute temperature. Mapping the particle temperature into cells, and exchange the cell

temperature according to the thermal diffusion.

(6) Re-distribute particles. Check the particle distribution and re-distribute particles when necessary, or put new particles into the inlet region according to the inlet boundary conditions.

The marker particles introduced into this calculation are only for the purpose of indicating fluid configuration, more specifically, helping to compute the liquid level-set value. With the liquid level-set value computed, the free surface of the liquid could be described more precisely.

Lagrangian Interpolation for Free Surface

When a free surface does not pass through the center of the cell, the second derivative of pressure φ in Eq. (3) should be taken carefully, the traditional differential process for the uniform grid will not be accurate enough. As a brief description, see Fig. 1. Let Φ denotes the level set value, the free surface with $\Phi = 0$ passes between point x_{k-1} and point x_k, and the applied pressure is φ_a. As x_{k-1} lies out the liquid, it cannot be applied to decide the grad of φ at point k because of discontinuity. Instead, we use x_a, x_k and x_{k+1} to construct a second order Lagrangian interpolation for φ:

$$\varphi(x) = \frac{(x-x_k)(x-x_{k+1})}{(x_a-x_k)(x_a-x_{k+1})}\varphi_a + \frac{(x-x_a)(x-x_{k+1})}{(x_k-x_a)(x_k-x_{k+1})}\varphi_k + \frac{(x-x_a)(x-x_k)}{(x_{k+1}-x_a)(x_{k+1}-x_k)}\varphi_{k+1} \tag{6}$$

and take its second derivative with respect to x gives

$$\frac{d^2\varphi}{dx^2} = \frac{2}{(x_a-x_k)(x_a-x_{k+1})}\varphi_a + \frac{2}{(x_k-x_a)(x_k-x_{k+1})}\varphi_k + \frac{2}{(x_{k+1}-x_a)(x_{k+1}-x_k)}\varphi_{k+1} \tag{7}$$

On the right side of Eq. (7), only x_a is to be decided, which can be estimated by level set value of its adjacent cell centers:

$$x_a = \frac{x_{k-1}\Phi_k - x_k\Phi_{k-1}}{\Phi_k - \Phi_{k-1}} \tag{8}$$

The Lagrangian interpolation as shown by Eq. (7) and Eq. (8) can be easily extended to two-dimensional or three-dimensional cases.

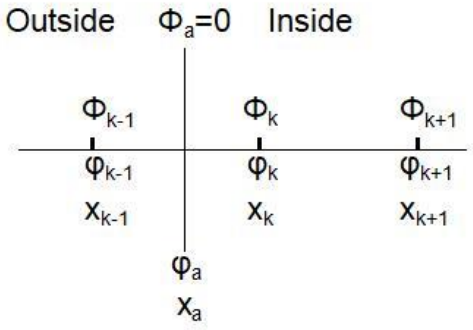

Fig. 1. One-dimensional schematic for free surface passes between cell centers

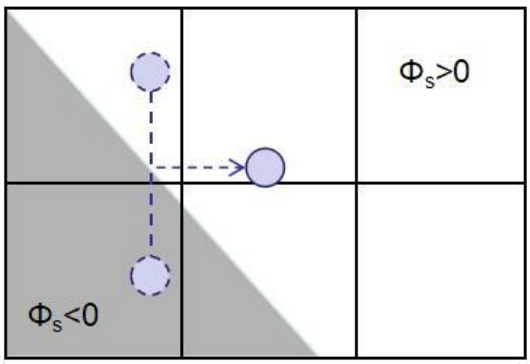

Fig. 2. Using level set to define oblique wall. The value inside the wall is negative while positive outside the wall.

Level set for the wall

The geometry of the casting is usually very complicated, involving many bevels and complex surfaces, which cannot be properly expressed using a simple uniform grid. For example, as Fig. 2 shows, an oblique wall blocks a dropping particle and deflects it to the right. If a simple uniform grid is used, because no oblique wall is defined, the particle will be reflected back up, not to the right. To handle this problem, one can preserve a level set field Φ_s for the solid wall, which is defined at the cell corner rather than the cell center. Φ_s is usually a signed distance field to the wall surface that computed when meshing the geometry. At the convection step [step (3)], whenever a particle runs to a new position $\vec{x}^*$, compute its solid level set value $\Phi_s(\vec{x}^*)$. If this value is negative ($\vec{x}^*$ inside the solid), a reflection operation should be taken:

$$\vec{x}^{n+1} = \vec{x}^* - (1+\alpha)\Phi_s(\vec{x}^*)\cdot\frac{\nabla\Phi_s(\vec{x}^*)}{|\nabla\Phi_s(\vec{x}^*)|} \tag{9}$$

In Eq. (9), the collision coefficient α should between 0 and 1. When $\alpha = 1$ a completely elastic collision strategy is applied, and $\alpha < 1$ applies an inelastic collision at the normal direction of the wall surface.

Examples and Applications

Collapse of a water column

The collapse of a water column was calculated with the parameters listed in table 1, and the geometry is depicted in Fig. 3. This geometry refers to the article of Koshizuka and Oka[10], because they had carried out an experiment[17]. In the experiment, a removable board supports the initial water column, and then it is pulled up within 0.05s and collapse starts. In our calculation, the pulling process of the board is neglected. In addition, we have also calculated this case with a VOF (Volume of Fluid) method using the same discrete procedure, and the same grid resolution. The results are shown in Fig. 4, cells with fluid are visualized rather than particles, in order to make a better comparison to the VOF method.

As shown in Fig. 4, at the beginning of the collapse, both methods have similar results. At t=0.24s, the results of the two calculations are slightly different. The fluid calculated by the MAC based method flows a bit faster than the VOF based method. It seems that the fluid calculated by VOF based method exhibits a greater viscosity. And by t=0.50s, the fluid interface calculated by the two methods is very different. From the MAC based method, we can see that the water hits the wall and breaks into pieces, forms very sharp and discontinuous interfaces. From the VOF based method, the water has smooth and continuous interfaces, which is not so real when referred to the experiment results.

Table. 1. Calculation parameters

Parameters	Value
Horizontal grid resolution	292
Vertical grid resolution	146
Particles per cell	4
Particle radius	$1.732\,\delta x$
Particle collision coefficient	$\alpha = 0$
Courant condition	$u_{\max}\delta t / \delta x \le 0.5$
Maximum time step	$\delta t \le 10^{-3} s$

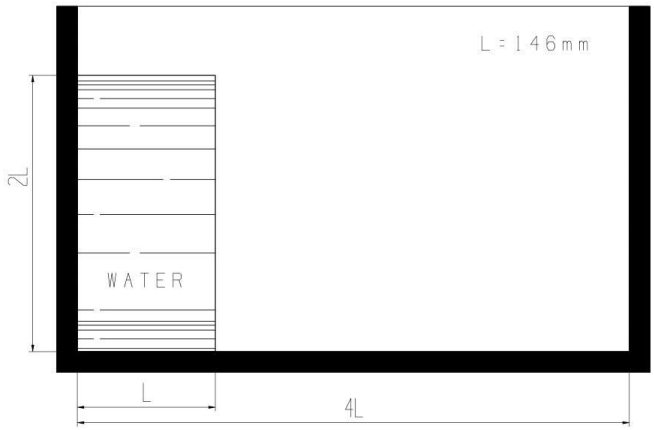

Fig. 3. Geometry of collapse of a water column

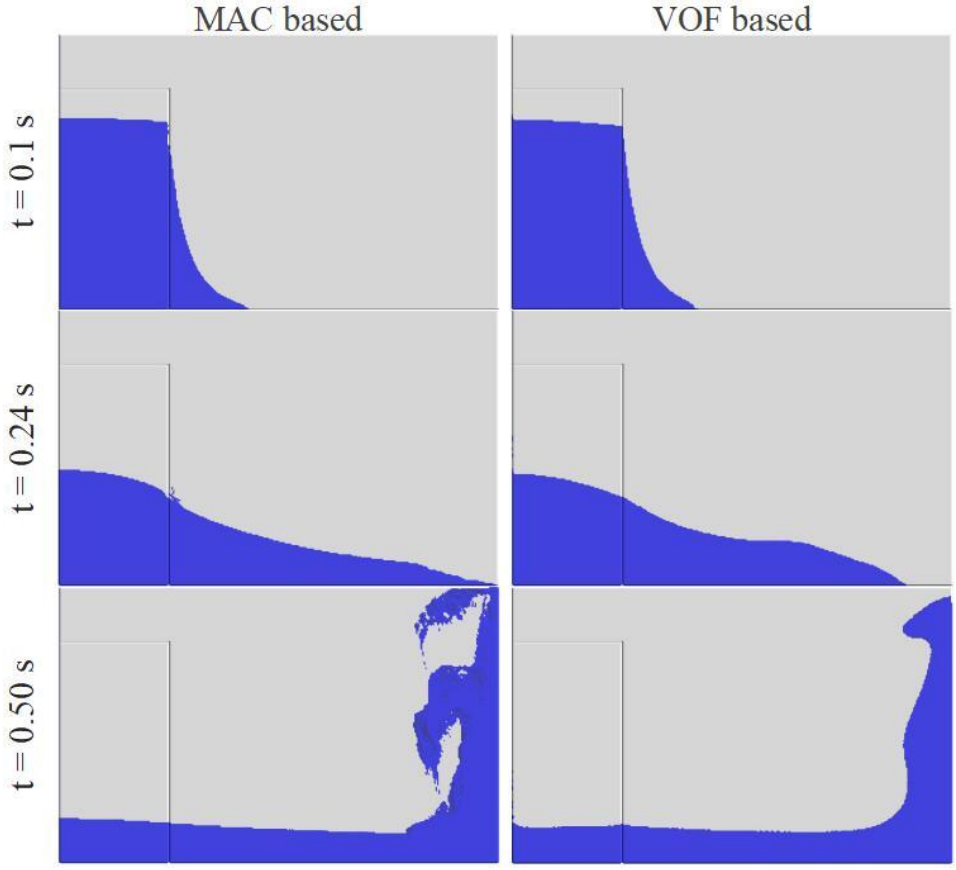

Fig. 4. Collapse of a water column calculated with MAC based method and VOF based method

Filling of a complex casting

The filling process of a practical iron casting scheme was calculated to study the application of this method. The simulation results were compared to results that calculated by a VOF program. Fig. 5(a) shows the geometric model of the investment casting system. The overall dimensions of the system are 200mm×100mm×500mm. There are four main sprues, each with 8 castings evenly distributed. The grid resolutions are 100×50×250, and there are a total of 1.25 million cells on the solution domain. In each cell, only 6 particles are placed for the sake of efficiency. Table. 2 shows the calculation parameters.

Table. 2. Parameters needed for the iron casting

Parameters	Value
Liquid iron density (kg/m^3)	6800
Liquid iron dynamic viscosity (Pa·s)	4.98e-3
Liquid iron specific heat (kJ/(kg·K))	0.82
Liquidus temperature (℃)	1500
Solidus temperature (℃)	1429
Latent heat (kJ/kg)	250
Acceleration of gravity (m/s^2)	(0, 0, -9.8)
Inlet temperature (℃)	1700
Inlet velocity (m/s)	0.15

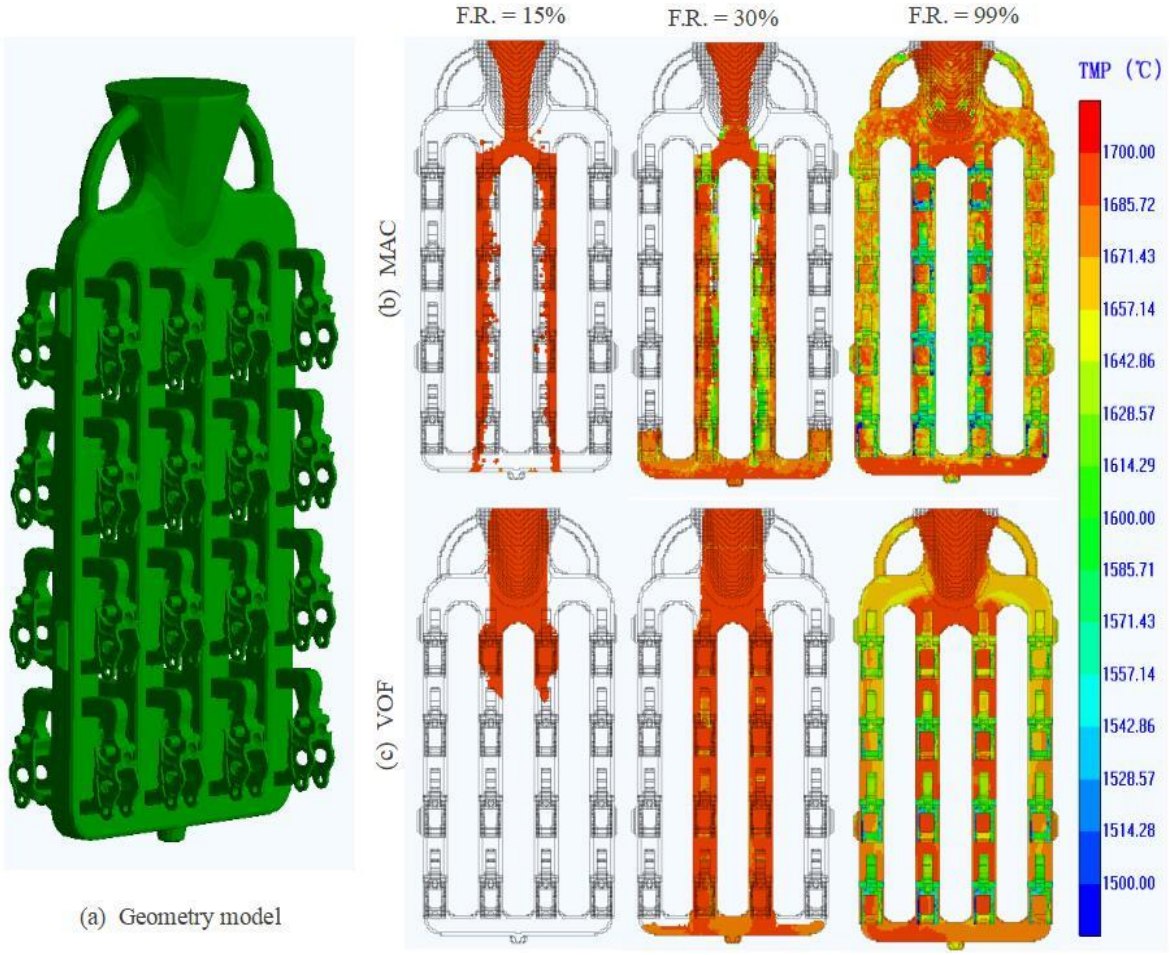

Fig. 5. Simulation of a complex casting filling process

Fig. 5(b) shows the results given by a MAC based method and Fig. 5(c) shows the results given by a VOF based method. After flowing into the casting system from the top of the pouring cup, the molten metal accelerates down until it hits the wall, and then diverts into two streams and continues to accelerate downward along the two inner sprues. Note that the molten metal will not fill the sprues at this moment, because the sum of the section areas of the inner sprues is larger. When these two streams reach the bottom of the system, they spread out symmetrically along the runner, and then enter the two outside sprues under the effect of pressure. At last, the castings start to be filled from bottom to top.

Both methods give the correct results, but the VOF based method gives a coarser stream in the early stage of the filling process as if the molten metal suffers a large surface tension, which is not so real. The MAC based method gives a better-looking stream. For the temperature filed, VOF based method gives a smoother distribution, and the MAC based method gives a mushy local temperature distribution, seems that the flow is more turbulent. This phenomenon may be caused by the re-distributing process. The particles have a tendency to gather together after a long run, and the re-distributing process must be carried out even though extra errors are introduced.

It takes 125 minutes to complete this simulation by the MAC based method using an Intel Core i7-6700HQ CPU, with an 8.0GB RAM. While the VOF based method takes only 98 minutes. That is to say, keeping track of the particles, takes not only more space, but also more time. This is a shortcoming of the MAC based method. However, with the particles tracked, something more complicated could be described, such as the oxide inclusions, the rising of slags in the mushy phase, which requires further research.

Conclusion

In this paper, the marker-and-cell method is introduced to simulate the casting filling process. The level set technique is used to enable the description of the complicated free surface and wall boundary, in a simple uniform grid. This MAC based method tracks the fluid surface directly by the marker particles, requires not only more storage space but also more calculation time than the VOF based method. However, it produces very sharp and discontinuous interfaces easily, which is a really pleasing property that suits the casting process with high flowing speed. Besides, with the particles tracked, some difficult problems like the oxide inclusions and the sand washing problems could become easier to be described.

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