Numerical Analysis on the Vortex Pattern and Flux Particle Dispersion in KR Method Using MPS Method

N Hirata¹, Y Xu¹ and K Anzai¹
¹ Department of Materials Processing, Graduate School of Engineering, Tohoku University, Sendai 980-8579, Japan

E-mail: hirata@material.tohoku.ac.jp

Abstract. The mechanically-stirring vessel is widely used in many fields, such as chemical reactor, bioreactor, and metallurgy, etc. The type of vortex mode that formed during impeller stirring has great effect on stirring efficiency, chemical reacting rate and air entrapment. Many efforts have been made to numerically simulate the fluid flow in the stirring vessel with classical Eulerian method. However, it is difficult to directly investigate the vortex mode and flux particle dispersion. Therefore, moving particle semi-implicit (MPS) method, which is based on Lagrangian method, is applied to simulate the fluid flow in a KR method in this practice. Top height and bottom heights of vortex surface in a steady state under several rotation speed was taken as key parameters to compare the results of numerical and published results. Flux particle dispersion behaviour under a rotation speed range from 80 to 480 rpm was also compared with the past study. The result shows that the numerical calculation has high consistency with experimental results. It is confirmed that the calculation using MPS method well reflected the vortex mode and flux particle dispersion in a mechanically-stirring vessel.

1. Introduction

Before continuous casting process, pre-treatment of melt is carried out to control a material components. Because of its good efficiency of liquid/solid and liquid/liquid mixing, mechanically-stirring vessel has been applied to improve the efficiency of chemical reacting for a long time [1-2]. The relationship between the pattern of stirring and efficiency of mixing [3-5], mass transfer [6-8], dissolution [9], precipitation [10] etc. has been studied subsequently. The mechanically-stirring method was firstly introduced to steelmaking industry by Kanbara et al. [11], in order to improve the efficiency of desulfurization reaction rate of melt and flux. It is still the major method in steel plants of Japan even now [12]. However, the melt and the vessel is opaque, and it is difficult to observe what happens during the operation. Therefore, enough but excess desulferization agent tends to be used for the process. To reduce the use of desulferization agents, many model experimentals have been conducted using water and floating materials to understand the flux dispersion behavior in the process. Nakai et al.[13] conducted experiment to investigate the flux dispersion behaviour during the desulfurization process in steelmaking process and proposed models to evaluate the particle size of desulfurization slag. They revealed that the flux dispersion is divided into three stages, non-dispersion, transition and complete dispersion, respectively, and the desulfurization rate of each stage is strongly related to the vortex mode.

Numerical analysis of single-phase and multi-phase flow in a mechanically-stirring tank or vessel has been reported by many researchers [1-2]. Most of them are based on the conventional Eulerian algorithm. For liquid/solid flow, some of the work was carried out with Eulerian algorithm for liquid flow coupling with Lagrangian algorithm for solid particle dispersion. However, most of the researches done with Eulerian algorithm focused on the velocity or pressure field in the fluid, and a few of them report the investigation on vortex mode in a stirring vessel.
Recently, the moving particle semi-implicit (MPS) method has been popularly discussed by researchers on the field of fluid flow. MPS method was firstly proposed by Koshizuka et al [14]. And ever since then, this meshless numerical simulation method based on Lagrangian algorithm has been widely studied because of its applicability for multi-phase flow with free surface. In this practice, the MPS method was applied to investigate the vortex pattern and particle dispersion in a mechanically-stirring vessel. The vortex height and particle dispersion results of numerical calculation were discussed with published results subsequently.

2. Numerical method

2.1. The MPS method

2.1.1. Weight Function

In the MPS method, governing equations consist of particle interaction equations. All interactions between particles are limited to a finite distance. The strength of interaction can be described using a weight function of distance between two particles. The gradient or other operators can be described using the weight function. Whereas numerous types of weight function have been proposed, equation (1) was used in this study [15].

\[
\begin{align*}
    w&(r, c_k r_0) = \begin{cases} 
      40 \frac{1}{7.2^3 \pi c_k} \left( 1 - 6 \left( \frac{r}{c_k r_0} \right)^2 + 6 \left( \frac{r}{c_k r_0} \right)^3 \right) & (0 \leq r < 0.5 c_k r_0) \\
      10 \frac{1}{7.2^3 \pi c_k} \left( 2 - 2 \frac{r}{c_k r_0} \right)^3 & (0.5 c_k r_0 \leq r < c_k r_0) \\
      0 & (c_k r_0 \leq r) 
    \end{cases}
\end{align*}
\]  

(1)

Here, \( r \) is the distance between the neighboring particles. \( r_0 \), which denotes the specific size of the particle, has the same significance as the lattice size in FDM. \( c_k \) is the kernel size coefficient and usually varies between 2 and 4. Particle number density \( n_i \) of the particle \( i \) is used in the MPS method to calculate the interaction between particle \( i \) and the surrounding particles. \( n_i \) is the sum of the weight function of the particles surrounding the particle \( i \), and is expressed as follows.

\[
n_i = \sum_{i \neq j} w\left( |r_j - r_i|, c_k r_0 \right)
\]

(2)

Here, \( r_i \) and \( r_j \) are the position vectors of particles \( i \) and \( j \), respectively. \( n_i \) is equal to \( n_0 \) in the case that a particle has no surface particle around it. Assuming that the fluid is incompressible and considering that the particle number density \( n_i \) is directly related to the fluid density, we can use \( n_0 \) for the mass conservation condition in the incompressible flow analysis using the MPS method.

2.1.2. Particle interaction models

Particle interaction models are used to describe differential operator in the particle method. If \( \phi_i \) and \( \phi_j \) are arbitrary scalars at positions \( r_i \) and \( r_j \), then the particle interaction models for the differential operators can be expressed as follows.

\[
\nabla \phi_i = \frac{d}{n_i} \sum_{i \neq j} \left( \phi_i - \phi_j \right) \frac{(r_j - r_i)}{|r_j - r_i|} w\left( |r_j - r_i|, c_k r_0 \right)
\]

(3)

\[
\nabla^2 \phi_i = \frac{2d}{n_i} \sum_{i \neq j} \left( \phi_i - \phi_j \right) \frac{(r_j - r_i)}{|r_j - r_i|^2} w\left( |r_j - r_i|, c_k r_0 \right)
\]

(4)
Equation (3) is a gradient model and equation (4) is a Laplacian model. Suffixes \( i \) and \( j \) represent the assigned numbers of particles. \( d \) is the number of space dimensions.

### 2.2. Fluid flow Analysis

The governing equations for incompressible flow consist of the continuity equation and Navier-Stokes equation as follows.

\[
\frac{D\rho}{Dt} = 0 \tag{5}
\]

\[
\frac{Du}{Dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 u + f \tag{6}
\]

Here, \( \rho \) indicates density (kg/m\(^3\)); \( u \), velocity vector (m/s); \( p \), pressure (Pa); \( \nu \), kinematic viscosity (m\(^2\)/s); and \( f \), the body force vector including gravity. Here, \( D/Dt \) is the symbol for Lagrangean differential equation without convection terms.

Flow calculation by the MPS method is based on the predictor-corrector method similar to that in the case of the FDM or other conventional methods. The major differences between the MPS method and the FDM are the formulation of the Poisson equation of pressure and the calculation of particle position. In the MPS method, the tentative particle position is calculated using tentative velocity in the prediction phase; therefore, the correction in position is calculated along with the correction in velocity in the correction phase. The Poisson equation for pressure in the MPS method is described using the tentative particle number density \( n^* \) and \( n_0 \) as follows. \( n^* \) is the particle number density calculated using the tentative particle positions.

\[
\nabla^2 p^{k+1} = -\frac{\rho}{\Delta t^2} \frac{n^* - n_0}{n_0} \tag{7}
\]

### 3. Hydrodynamic Experiment in Past Research

Hydrodynamic experiment and results published by Nakai et al. [13] are used to verify the numerical simulation by MPS method. As illustrated in Fig.1, a four-blade Rushton turbine is set in the center of the vessel with the whole impeller immersed in a certain depth \( L \). \( \Delta H_1 \) and \( \Delta H_2 \) are the differential value of vortex bottom height and top height from the initial water height \( H_0 \), respectively. Domain A and Domain B are defined as the left side in the sight of the space between the vessel wall and impeller blades, so that the particle dispersion could be studied in these two domains. The boundary to separate these two domains is the central line of the initial water height. The numerical calculation at \( L=214\)mm and \( L=338\)mm are carried out. The results at different rotation speed (RS), varying from 80 to 480 rpm, are obtained numerically to compare with past experimental results by Nakai et al. Nakai et al. counted the number of particles in domain A and domain B after reaching steady state by evaluating the interfacial area between the particles and water using image processing method.

Table1 gives the vessel size and stirring information in the research by Nakai et al. and numerical analysis in this study. The calculation conditions are same as published research. Only flux density is different because of the calculation stability.
Table 1. Hydrodynamic experiment conditions.

| Item                        | Water model by Nakai et al. [13] | Numerical simulation (this study) |
|-----------------------------|-----------------------------------|----------------------------------|
| Vessel Height               | 695mm                             | 695mm                            |
| Diameter                    | 523mm                             | 523mm                            |
| Water Depth \((H_0)\)       | 414mm                             | 414mm                            |
| Rotation Speed \((RS)\)     | 80–480rpm                         | 80–480rpm                        |
| Impeller Height             | 110mm                             | 110mm                            |
| Diameter                    | 203mm                             | 203mm                            |
| Width                       | 52mm                              | 52mm                             |
| Impeller Immersion Depth \((L)\) | 214mm, 338mm                   | 214mm, 338mm                     |
| Particle Density            | 0.03g/m³                          | 0.5g/m³                          |

4. Results and discussions

4.1. Vortex Height
There are two critical heights for the vortex, \(\Delta H_1\) and \(\Delta H_2\) as shown in figure 1. Figure 2 shows numerical results of \(\Delta H_1\) and \(\Delta H_2\) variation with rotation speed and compares that with reported data by Nakai et al\(^{13}\). \(\Delta H_1\) and \(\Delta H_2\) are measured after the flow behavior reaches to the steady state. As is illustrated in figure 2(a) and figure 2(b), numerical results of \(\Delta H_1\) and \(\Delta H_2\) variation for \(L=214\) mm case with rotation speed match good with that reported by Nakai et al.. \(\Delta H_1\) is minor when \(RS\) is lower than 80 rpm, and increased fast to a steady level around 250 mm when \(RS\) grows up to 200 rpm. Numerical \(\Delta H_2\) variation also shows good agreement with the past study. It presents quasi-linear feature with \(RS\). Figure 2(c) and figure 2(d) are the results for the case of \(L=338\) mm. The calculated results coincide with the results in the past study quite well. The calculated \(\Delta H_1\) increases from about 10 mm at \(RS=80\) rpm to 414 mm (Vessel bottom) at \(RS=360\) rpm continuously. In the past study, \(\Delta H_1\) rises up to 414 mm at \(RS=320\) rpm. The comparison of numerical and reported experimental results on \(\Delta H_1\) and \(\Delta H_2\) variation shows that the numerical method well reflects the vortex mode in a mechanically-stirring vessel.
4.2. Relationship between the vortex mode and particle dispersion

There are three types of vortex mode in a mechanically-stirring vessel according to the relative position of the vortex bottom and the impeller, and the vortex mode correlates the rotation speed of the impeller [13]. Figure 3 is the schematics of vortex mode and the figure 4 shows the particle dispersion.
information of numerical results at steady state. As shown in Figure 3 and 4, the flux particle dispersion behavior is strongly related to the vortex mode. Mode I: Non-dispersion stage, the vortex bottom is higher than the impeller, in this stage, there is no particles dispersed in the water. Mode II: Transition stage, the vortex bottom is right on the height range of impeller and the particle dispersion emerges. Mode III: Complete dispersion stage, the vortex bottom in under the impeller and much air is entrapped; the particles disperse in the whole scale of the vessel.

In figure 4(a), which illustrates the particle dispersion for $L=214$mm case, very few particles enter the water at $RS=160$rpm. When the rotation speed goes up to 240rpm, a great amount of particles begin entering the water, as shown in figure 4(b). Finally, all of the particles enter the water as shown in figure 4(c), where $RS=320$rpm. Figure 4(d) to figure 4(f) shows the results in the case of $L=338$mm. No particle enters the water at 160 rpm rotation speed and a small number enters when the rotation speed grows up to 240 rpm. Even in 320 rpm, not all of the particles can enter the water. The mixing efficiency of 214mm impeller immersion depth is better than that of 338 mm impeller immersion depth according to the numerical results.

4.3. Particle dispersion in the domain A and B

In the study by Nakai et al.[13], the amount of particle dispersion in the domain A and B are counted by the method of evaluating the particle occupying area percentage in the picture. Figure 5 shows the counted particle numbers of numerical simulation in this study and past research done by Nakai et al. in domain A and B when the stirring status becomes steady state. The immersion depths of impeller are $L=214$mm and $L=338$mm. The particle size in the report by Nakai et al. was $2mm$, in contrast to $13mm$ in numerical simulation. As a result, the total particle number in numerical calculation in this study is fewer than that in the past research. This is also the reason why the vertical axises in figure 4 have different magnitude. In this discussion, the tendency of particle dispersion variation is compared.

![Figure 4](image-url)

**Figure 4.** Numerical simulation result of particle dispersion. 

Figure 5(a) and figure 5(b) is the calculated results of the number of flux particle counted in the domain A and B. When the impeller rotation speed is low and the vortex type is mode I, few particles are entrapped into the liquid. With the rotation speeding up, vortex type turns to mode II, massive particles are drawn into domain A both in $L=214$mm and $L=338$mm cases. However, there is no
obvious difference for that in domain B. If the rotation speed keeps growing up, particles are found to decrease for \( L=214 \text{mm} \) case and increase for \( L=338 \text{mm} \) case in domain A. The particle amount dramatically rises in domain B for \( L=214 \text{mm} \) case while it decreased to almost none for \( L=338 \text{mm} \) case.

Figure 5(c) and figure 5(d) show the water model experimental results by Nakai et al. [13]. In domain A, the particle amounts changing curve is quite similar to the numerical results for \( L=214 \text{mm} \) case while the \( L=338 \text{mm} \) case has some difference in mode III. Numerical results do not grow up as dramatically as experimental results do. In domain B, the amount of particles for \( L=214 \text{mm} \) case shows almost no change after the stirring turns to mode II in the experiment whereas the amount decreased to almost zero when the stirring turns to mode III in numerical results. Another difference is that the number of particles dispersed in domain B in the experimental results keeps a steady level when the rotation speed rises up to certain strength while that for numerical results keeps growing up.

One of the reason for the differences of particle dispersion behaviour in the domain A and B is that the air entrapment has not been considered in numerical analysis. In the actual experiment, much air entrapment emerged over \( RS=320 \text{rpm} \) according to the report by Nakai et al. The bubbles generate at high rotation speed are drawn into the deep area, and emerge the particles from the water.

Particle methods is suitable for the multi-phase and multi-physics calculation, therefore the proposed method can be extend to calculate not only the flux dispersion behavior, but chemical reaction and efficiency of desulferization. As a result, significant contribution is expected in the reduction of the desulferization agent consumption. In addition, the results in this study show that the proposed method can capture the dispersion behavior of flux without numerical diffusion. This advantage is also expected in capturing the behavior of inclusions or bubbles in the continuous casting process, by which considerable defects occurs.

![Figure 5](source.png)

**Figure 5.** Relationship between number of particles and rotation speed.
5. Conclusions
MPS method was applied to analyze fluid flow in a mechanically-stirring vessel in this paper. Numerical results of particle dispersion in domain A and B and the differential of vortex top height and bottom height with initial water height, named as $\Delta H_1$ and $\Delta H_2$, were compared with past report by Nakai et al. The comparison shows that the numerical method reflected the vortex pattern well.

The numerical results of particle dispersion in the water present consistency with Nakai et al.’s report. In the first stage of stirring, there is no or few particles enter the water. The amount of particles entrapped into the water increase with the rotation speed growing up and totally be entrapped finally. Particle amounts in certain domains are also counted to compare with past research; the numerical results of particle amount variation have relative consistency with that of past research. There are some differences between numerical particle dispersion results in domain A and domain B. It is attributed to the neglecting of air entrainment in numerical analysis.

References
[1] Joshi J B, Nere N K, Rane C V, Murthy B N, Mathpati C S, Patwardhan A W, and Ranade V V 2011 *The Canadian Journal of Chemical Engineering*, 89 23
[2] Joshi J B, Nere N K, Rane C V, Murthy B N, Mathpati C S, Patwardhan A W, and Ranade V V 2011 *The Canadian Journal of Chemical Engineering*, 89 754
[3] Ochieng A, Onyango M S, Kumar A, Kiriamiti K, Musonge P 2008 *Chemical Engineering and Processing* 47 842
[4] Guillard F, Tragardh C 2003 *Chemical Engineering and Processing* 42 373
[5] Kasat G R, Khopkar A R, Ranade V V, Pandit A B 2008 *Chemical Engineering Science*, 63 3877
[6] Martin M, Montes F J, Galán M A 2010 *Chemical Engineering Science* 65 3814
[7] Kerdouss F, Bannari A, Proulx P, Bannari R, Skrga M, Labrecque Y 2008 *Computers and Chemical Engineering* 32 1943
[8] Brüning S, Weuster-Botz D 2014 *Chemical Engineering Research and Design* 92 240
[9] Hartmann H, Derksen J J, Akker H.E.A. van den 2006 *Chemical Engineering Science* 61 3025
[10] Jaworski Z, Nienow A W 2003 *Chemical Engineering Journal* 91 167
[11] Kanbara K, Nisugi T, Shiraishi O, Hatakeyama T 1972 *Tetsu-to- Hagané* 58 34
[12] Ogawa Y, Maruoka N 2014 *Tetsu-to- Hagané* 100 434
[13] Nakai Y, Sumi I, Matusno H, Kikuchi N, Kishimoto Y 2010 *ISIJ International* 50 403-410
[14] Koshizuka S, Oka Y 1996 *Nuclear Science and Engineering* 123 421
[15] Hirata N, Anzai K 2011 *Journal of Japan Foundry Society* 83 259