Numerical Simulation of Rayleigh-Taylor Instability by Multiphase MPS Method

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***Abstract*—The Rayleigh-Taylor instability problem is one of the classic hydrodynamic instability cases in natural scenarios and industrial applications. For the numerical simulation of the Rayleigh-Taylor instability problem, this paper presents a multiphase method based on the moving particle semi-implicit (MPS) method. Herein, the incompressibility of the fluids is satisfied by solving a Poisson Pressure Equation and the pressure fluctuation is suppressed. A single set of equations is utilized for fluids with different densities, making the method relatively simple. To deal with the mathematical discontinuity of density in the two-phase interface, a transitional region is introduced into this method. For particles in the transitional region, a density smoothing scheme is applied to improve the numerical stability. The simulation results show that the present MPS multiphase method is capable of capturing the evolutionary features of the Rayleigh-Taylor instability, even in the later stage when the two-phase interface is quite distorted. The unphysical penetration in the interface is limited, proving the stability and accuracy of the proposed method.**

I. INTRODUTION

The Rayleigh-Taylor instability (RTI) is one of the most common instability phenomena existing in multi-fluid flows. Due to the density difference of different fluids, the two-phase interface is sensitive to various perturbation. Even a very small perturbation may induce a fingering RTI in which the light fluid violently pushes the heavy fluid against gravity. The RTI can be observed in a wide range of natural scenarios and industrial applications, including astrophysics, nuclear engineering, turbulent mixing, and inertial confinement fusion (ICF).

Due to the strong nonlinearity of the RTI, theoretical investigations have difficulties in obtaining correct results beyond the early linear regime. And experimental investigations are easily influenced by the perturbation introduced in the experimental process itself. In recent decades, the huge progress of Computational Fluid Dynamics (CFD) facilitates the application of a variety of numerical methods to the simulations of the RTI.

In the RTI simulations, the tracing of the two–phase interface is the most important technology. Compared with grid-based methods, the gridless particle methods is more advantageous for solving multiphase problems with large deformation of the two –phase interface. However, stable multiphase simulations is difficult to be conducted due to the discontinuity of density in the interface and the phenomenon of pressure fluctuation commonly existing in particle method. Therefore, a stable and accurate multiphase model in particle methods is necessary to be studied.

The moving particle semi-implicit (MPS) which is originally proposed by Koshizuka and Oka [1], is an important kind of particle method. By solving the Poisson Pressure Equation (PPE), the MPS method is suitable for the simulations of fully incompressible flow. The first MPS multiphase method is developed by Gotoh and Fredsøe [2] for solid-liquid two-phase flows. Liu et al. [3] proposed a hybrid MPS-FVM method for the viscous, incompressible, multiphase flows, in which the heavier fluid is represented by moving particles while the lighter fluid is defined on the mesh. Shakibaeinia and Jin [4] studied a straightforward multiphase method based on the weakly compressible MPS (WCMPS) method, by treating the multiphase system as a multi-viscosity and multi-density system, but the unphysical penetration is observed due to the weakly compressibility of their method, . Khayyer and Gotoh [5] firstly developed four schemes which are more accurate and consistent than the schemes of the original MPS method, then a first order density smoothing scheme [6] is derived for multiphase flows characterized by high density ratios. Although experiencing a much shorter development time than the grid-based methods, the MPS method has shown the advantages in multiphase simulations, especially when the large deformation of interface exists, such as the simulation of RTI.

In this paper, a MPS multiphase solver is developed and applied to the simulation of RTI. The multiphase solver is based on our in-house single phase particle method solver MLParticle-SJTU, and a density smoothing scheme is included for the treatment of two-phase interface. The MLParticle-SJTU solver adopts the modified MPS method and has been commonly applied to a variety of violent hydrodynamic problems, such as liquid sloshing flows [7-9], dam-breaking flows [10-12], wave-floating body interaction [13,14], water entry problems [15,16], fluid-structure interaction [17,18]. The density smoothing scheme here is similar with the scheme adopted by Shakibaeinia and Jin [4], in which the density discontinuity in the interface is avoided through setting a transitional region. In the next parts of this paper, the MPS multiphase method is firstly introduced in detail. Then, the simulation of RTI is conducted and the stability and accuracy of the MPS multiphase method is validated.

II. NUMERICAL SCHEME

A. Governing Equations

In the present method, the multiphase system is treated as a multi-density system. The form of governing equations for different fluids is identical, written as:

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{V} = 0 \tag{1}$$

$$\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla\cdot P + \nu\nabla^2\cdot\boldsymbol{V} + \boldsymbol{g} \tag{2}$$

where $\boldsymbol{V}$ is the flow velocity vector, P is the pressure, ρ is the fluid density, ν is the kinematic viscosity, $\boldsymbol{g}$ is the gravitational acceleration vector. For different fluids, the ρ and ν in above equations are different. Differing from the governing equations in grid-based methods, the convective acceleration term in the left hand side of momentum conservation equation is included in the material derivative, thus the numerical diffusion is eliminated.

B. Kernel Function

The spatial derivatives in the governing equation need to be approximated by the particles interaction. A particle interacts with all particles within a specified domain. The size of this domain is defined as the radius of the interaction area of each particle. To weight the interaction of each pair of particles, a kernel function is introduced in the MPS method. This article adopts a modified kernel function proposed by Zhang and Wan [13], which can be written as:

$$W(r_{ij}) = \begin{cases} \dfrac{r_e}{0.85r_{ij}+0.15r_e} - 1 & \left(0 \le r_{ij} < r_e\right) \\ 0 & \left(r_e \le r_{ij}\right) \end{cases} \tag{3}$$

where r_{ij} is the distance between particle i and particle j, r_e is the maximum radius of support region. Compared with the original kernel function proposed by Koshizuka [1], the modified kernel function prevents the existence of singular point by making the value of $W(r_{ij})$ finite when the r_{ij} is equal to zero. Thus the numerical instability of the MPS method can be improved.

C. Gradient Model

In the MPS method, the gradient operator is discretized into a local weighted average of radial function. In this paper, an anti-symmetric gradient model is adopted, written as:

$$\langle\nabla P\rangle_i = \frac{d}{n^0}\sum_{j\neq i}\left[\frac{P_j - P_{i\_\min}}{\left|\boldsymbol{r}_j - \boldsymbol{r}_i\right|^2}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right)\cdot W(r_{ij})\right] \tag{4}$$

where $\langle\ \rangle_i$ represents the kernel approximation in particle i, n^0 represents the initial particle number density, d is the number of space dimension, $P_{i\_\min}$ refers to the minimum pressure within the support domain of particle i. This model is proposed by Koshizuka [19], to overcome the tensile instability of original model by ensuring repulsive force between particles.

D. Laplacian Model

The Laplacian model used here is derived by Koshizuka [1] from the physical concept of diffusion, written as:

$$<\nabla^2\phi>_i = \frac{2d}{n^0\lambda}\sum_{j\neq i}(\phi_j - \phi_i)\cdot W(r_{ij}) \tag{5}$$

$$\lambda = \frac{\sum_{j\neq i} W(r_{ij})\cdot|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}{\sum_{j\neq i} W(r_{ij})} \tag{6}$$

where λ is a parameter introduced to keep the increase of variance equal to analytical solution.

E. Model of Incompressibility

In order to keep the fluids incompressible, a semi-implicit algorithm is employed in the MPS method. The main characteristic of this algorithm is the prediction-correction process in each iteration. In the prediction step, a temporal velocity is explicitly predicted based on the gravity term and viscosity term as follow:

$$\boldsymbol{V}_i^* = \boldsymbol{V}_i^k + \Delta t(\nu\nabla^2\cdot\boldsymbol{V} + \boldsymbol{g}) \tag{7}$$

Since the temporal velocity field doesn't satisfy the divergence-free condition, a second correction step is required to project the velocity field into a divergence-free space. The velocity is corrected based on the pressure gradient as follow:

$$\boldsymbol{V}_i^{k+1} = \boldsymbol{V}_i^* - \frac{\Delta t}{\rho}\nabla P^{k+1} \tag{8}$$

In the MPS method, the pressure field is obtained by solving the Poisson Pressure Equation (PPE). To suppress the pressure oscillation, we employ the PPE with the mixed source term of constant particle number density condition and divergence-free condition. This is developed by Tanaka and Masunaga [20] and rewritten by Lee [21] as:

$$\left\langle \nabla^2 P^{k+1} \right\rangle_i = (1-\gamma)\frac{\rho}{\Delta t}\nabla \cdot \boldsymbol{V}_i^* - \gamma \frac{\rho}{\Delta t^2}\frac{\left\langle n^k \right\rangle_i - n^0}{n^0} \quad (9)$$

where γ is a parameter suggested to be 0.01, the superscripts k and $k+1$ indicate the current time step, $\left\langle n^k \right\rangle_i$ represents the particle number density at k^{th} time step.

F. Density Smoothing

When the particle methods are employed to simulate the multiphase flows, a major challenge is the density discontinuity in the two-phase interface, which would result in an unsmooth pressure gradient field. This is the main reason of the interface disorder and the blow-up of simulation.

To overcome this problem, we adopt a density smoothing method similar with the one used by Shakibaeinia and Jin [4]. In this method, a transitional region is introduced to smooth the densities of particles within a certain distance (the width of density smoothing) from the interface. The densities of these particles are re-evaluated according to a spatial averaging of the densities of all neighbouring particles. The spatial averaging follows the formula below:

$$\left\langle \rho \right\rangle_i = \frac{\sum_{j \neq i} \rho_j \cdot W(r_{ij})}{\sum_{j \neq i} W(r_{ij})} \quad (10)$$

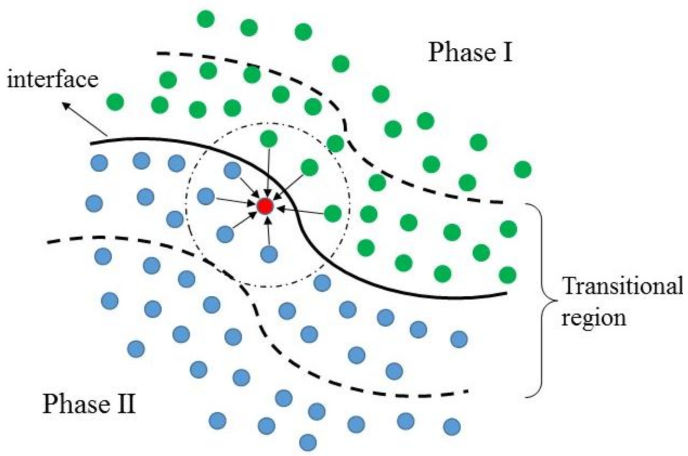

Figure 1. Sketch of density smoothing

The results obtained by Shakibaeinia and Jin [4] have validated the reliability of the density smoothing scheme. However, there still be some unphysical penetration being observed in the interface, even in the early stage when the motion of particles is not violent. This may be induced by the weakly compressibility of the WCMPS method used in their study. In this paper, we employ a fully incompressible MPS, which has been proven to be effective to suppress the pressure fluctuation. Therefore, the density smoothing scheme is believed to be enough to deal with the density discontinuity in the two-phase interface.

III. NUMERICAL SIMULATION

A. Numerical Setup

In this part, we consider the RTI problem in a rectangular container with the dimension of 0.5 m (width) × 1 m (height), as illustrated in Fig. 2. The origin of coordinates is fixed in the middle point of this container. The heavier fluid is identified by the Green color, with a density of 3000 kg/m^3. The lighter fluid is identified by the blue color, with a density of 1000 kg/m^3. The interface of these two fluids is given an initial single mode perturbation, $y_{\text{interface}}$ = 0.025cos(4πx). The gravity acceleration in this simulation is set to be g=10 m/s and points downwards. To better test the stability of this method, the viscous effect is ignored in our simulation. The initial particle distance r_0 is 0.005 m, meaning that totally 100 × 200 fluid particles are used in our simulation. In the MPS method, the radiuses of the interaction area for different models don't need to be quite the same. For the purpose of saving computational cost, the radius of the interaction area for gradient model and the width of density smoothing is 4.1r_0, the radius of the interaction area for Laplacian model is 8.1r_0 in our simulation.

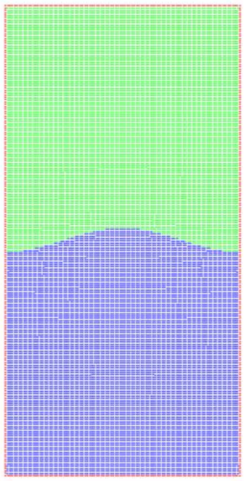

Figure 2. Initial distribution of particles

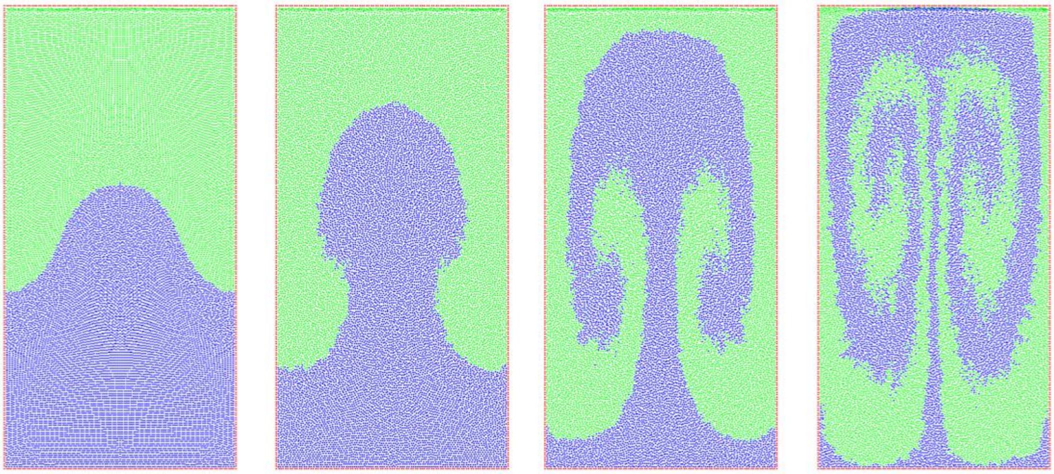

Figure 3. Evolution of RTI with a density ratio of 3:1, at *t* = 0.5 s, 1 s, 1.5 s, 2 s.

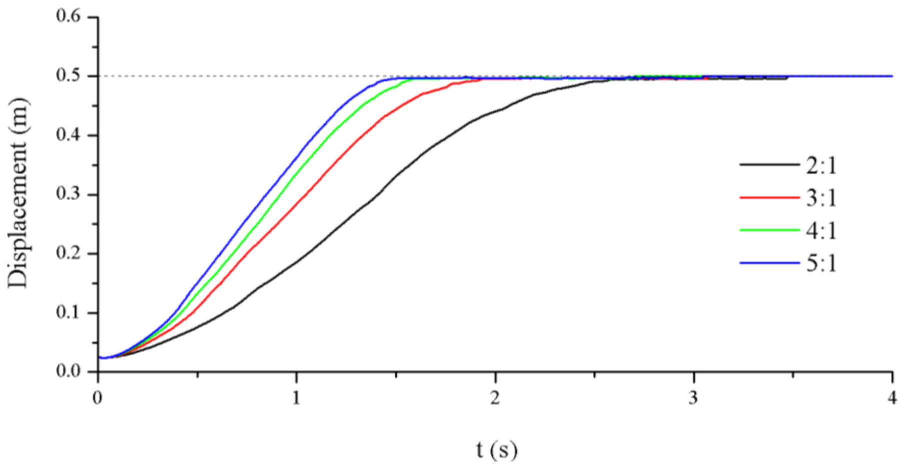

Figure 4. Displacement of the peak of the lighter fluid with different density ratios.

B. Results

Fig. 3 shows the evolution of the RTI problem with a density ratio of 3:1 at 0.5 s, 1 s, 1.5 s, 2 s. The simulation snapshot of the simulation demonstrates the ability of the present MPS multiphase method to capture the complex interface between two different fluids. Under the effect of initial perturbation, the lighter fluid moves upward and pushes the heavier fluid upon, then a bubble is formed at 0.5 s. After about 1 s, the upside part of the lighter fluid starts to form a mushroom shape. At 1.5 s, due to the influence of the neighbouring heavier fluid moving downward, two streams of the lighter fluid are separated from the rising part and strong vortex roll can be observed. At 2 s, the vortex roll becomes stronger and the light fluid reaches the top of the container. The evolution of RTI is similar with the results obtained by Shakibaeinia and Jin [4] at early stage, but due to ignorance of viscous effects in our simulation, more of the lighter fluid are able to move upward, resulting in a more complex vortex structure. And the unphysical penetrations in our simulation are much less compared with the results obtained by Shakibaeinia and Jin [4] with a large kinematic viscosity of 0.01.

Fig. 4 compared the growth rate of RTI with different density ratios. When the density ratio increasing from 2:1 to 5:1, the time needed for the lighter fluid to reach the top of the container is largely reduced, indicating the importance of the density ratio for RTI problems. This also illustrates the applicability of the present MPS multiphase method for multiphase flows with different density ratios.

Fig. 5 shows the velocity vector of all particles in the RTI simulation. An obvious symmetry property can be observed during the whole RTI evolution process. Two vortexes appear respectively at the two balanced positions of the initial perturbation at 0.5 s, which is induced by the interaction of upward motion of the lighter fluid and downward motion of the heavier fluid. Then these vortexes keep developing fast and forms multilayer vortex with clear two-phase interface at 2 s. Moreover, another two vortexes appear near the corner in the bottom of the container at 2 s, complicating the flow field structure.

Fig. 6 and Fig. 7 demonstrate the y-velocity and x-velocity during the simulation, respectively. In y-direction, the velocity of middle part of the fluid field points upside, just the reverse for the fluid near two side walls. In x-direction, the fluid near the bottom converges toward the middle of the tank, while the fluid near the top separately flows to two side walls.

IV. CONCLUSION

The paper proposes a MPS multiphase method and develops corresponding solver based on our in-house single phase particle method solver MLParticle-SJTU. When the multiphase solver is applied to the simulation of Rayleigh-Taylor instability, stable and accurate results can be obtained. The density smoothing scheme used in this paper can greatly reduce the unphysical penetrations appearing in other multiphase methods and keep the two-phase interface clear and natural, even when the interface is quite distorted. The results show that the complete evolution of Rayleigh-Taylor instability when an initial perturbation is given to the interface position. At the beginning, the lighter fluid pushes upon the heavier fluid and forms a mush-like shape. Two vortexes appear and develop fast to become the main flow characteristic in the container. Another two vortexes appear in the later time, indicating the complexity of the RTI problems. The simulations of RTI with different density ratios demonstrate the important role of the high density ratio in improving the growth rate of RTI, and validate the applicability of the MPS multiphase method in different conditions.

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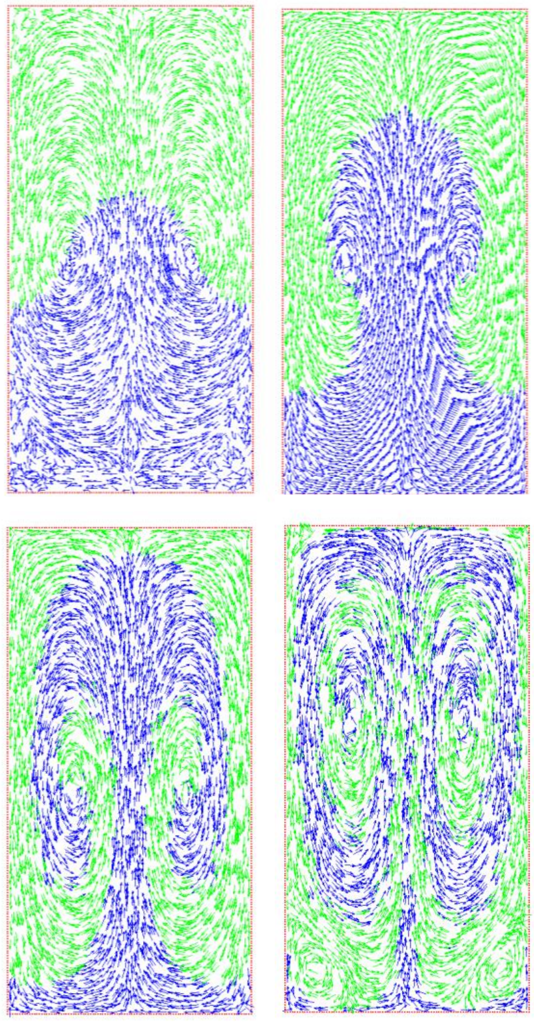

Figure 5. Velocity vector of RTI with a density ratio of 3:1, at t = 0.5 s, 1 s, 1.5 s, 2 s

REFERENCES

[1] S. Koshizuka and Y. Oka, "Moving-particle semi-implicit method for fragmentation of incompressible fluid," Nuclear Science & Engineering, vol. 123(3), pp. 421-434, 1996.

[2] H. Gotoh and J. Fredsøe, "Lagrangian two-phase flow model of the settling behavior of fine sediment dumped into water," Proc. ICCE, Sydney, pp. 3906–3919, 2000.

[3] J. Liu, S. Koshizuka, and Y.Oka, "A hybrid particle-mesh method for viscous, incompressible, multiphase flows," Journal of Computational Physics, vol. 202(1), pp. 65-93, 2005.

[4] A. Shakibaeinia and Y. C. Jin, "MPS mesh-free particle method for multiphase flows," Computer Methods in Applied Mechanics & Engineering, vol. 229, pp. 13-26, 2012.

[5] A. Khayyer and H. Gotoh, "Enhancement of stability and accuracy of the moving particle semi-implicit method," Journal of Computational Physics, vol. 230, pp. 3093-3118, 2011.

[6] A. Khayyer and H. Gotoh, "Enhancement of performance and stability of MPS mesh-free particle method for multiphase flows characterized by high density ratios," Journal of Computational Physics, vol. 242, pp. 211-233, 2013.

[7] X. Wen, X. Chen, and D. C. Wan, "MPS simulation of sloshing flows in a tuned liquid damper," Proceedings of the Twenty-seven International Ocean and Polar Engineering Conference, San Francisco, USA, pp. 1009-1016, 2017.

[8] Y. X. Zhang and D. C. Wan, "Comparative study of MPS method and Level-Set method for sloshing flows," Journal of Hydrodynamics, vol. 26(4), pp. 577-585, 2014.

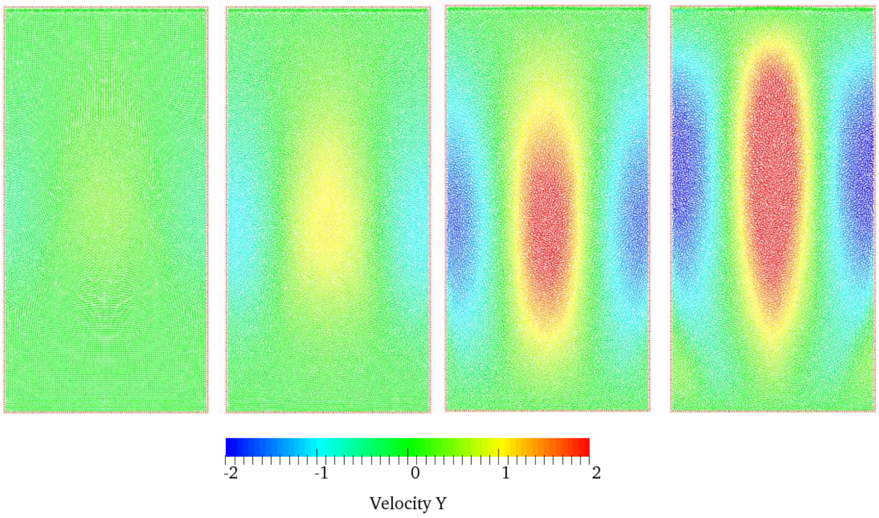

Figure 6. Y-velocity of RTI with a density ratio of 3:1 , at t = 0.5 s, 1 s, 1.5 s, 2 s.

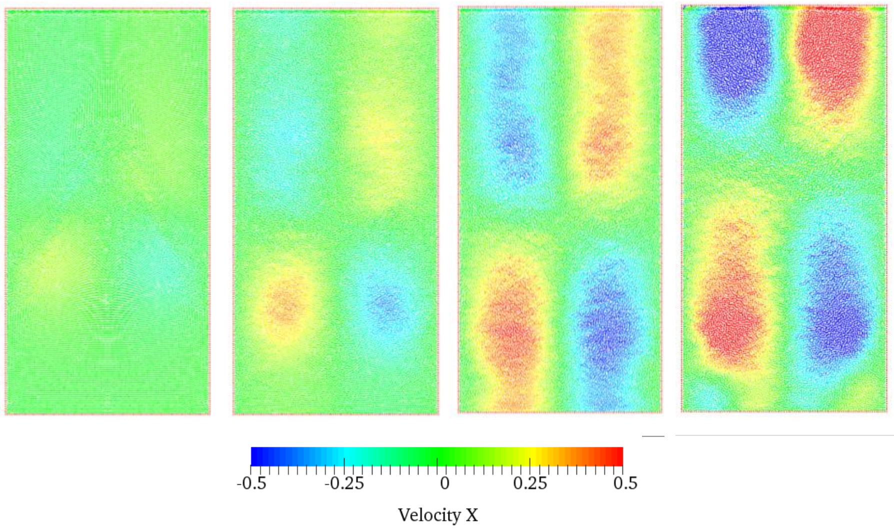

Figure 7. X-velocity of RTI with a density ratio of 3:1, at t = 0.5 s, 1 s, 1.5 s, 2

[9] X. Chen, Z. Y. Tang, and D. C. Wan, "The effects of T type baffle on liquid sloshing by MPS method, Proceedings of 3rd International Conference on Violent Flows, Osaka, Japan, No. 25, 2016.

[10] Y. X. Zhang, "Application of MPS in 3D dam breaking flows," Scientia Sinica, vol. 41, pp. 140-151, 2011. (in Chinese)

[11] Z. Y. Tang, Y. L. Zhang, and D. C. Wan, "Multi-resolution MPS method for free surface flows," International Journal of Computational Methods, vol. 13(04), No. 1641018, 2016.

[12] Z. Y. Tang, Y. L. Zhang, and D. C. Wan, "Numerical simulation of 3-D free surface flows by overlapping MPS," Journal of Hydrodynamics, vol. 28(2), pp. 306-312, 2016.

[13] Y. L. Zhang and D. C. Wan, "Numerical study of interactions between waves and free rolling body by IMPS method," Computers and Fluids, vol. 155, pp. 124–133, 2016.

[14] Y. L. Zhang, Z. Y. Tang, and D. C. Wan, "Numerical investigations of waves Interacting with free rolling body by modified MPS method, " International Journal of Computational Methods, vol. 13(04), No. 1641013, 2016.

[15] X. Chen, C. P. Rao, and D. C. Wan, "Numerical simulation of water entry of two-dimensional wedge by MPS," Chinese Journal of Computational Mechanics, vol. 34(3), pp. 356-362, 2017.

[16] Y. L. Zhang, Z. Y. Tang, and D. C. Wan, "Simulation of water entry of a free-falling wedge by improved MPS method," Proceedings of the Twenty-sixth International Ocean and Polar Engineering Conference, Rhodes, Greece, pp. 220-227, 2016.

[17] Y. L. Zhang, X. Chen, and D. C. Wan, "MPS-FEM coupled method for the comparison study of liquid sloshing flows interacting with rigid and elastic baffles," Applied Mathematics and Mechanics, vol. 37(12), pp. 1359-1377, 2016.

[18] Y. L. Zhang, X. Chen, and D. C. Wan, "Sloshing flows in an elastic tank with high filling liquid by MPS-FEM coupled method," Proceedings of the Twenty-seven International Ocean and Polar Engineering Conference, San Francisco, USA, pp. 1077-1084, 2017.

[19] S. Koshizuka, A. Nobe, and Y. Oka, "Numerical analysis of breaking waves using the moving particle semi - implicit method," International Journal for Numerical Methods in Fluids, vol. 26(7), pp. 751-769, 1998.

[20] M. Tanaka and T. Masunaga, "Stabilization and smoothing of pressure in MPS method by quasi-compressibility," Journal of Computational Physics, vol. 229(11), pp. 4279-4290, 2010.

[21] B. H. Lee, J. C. Park, M. H. Kim, and S. C. Hwang, "Step-by-step improvement of MPS method in simulating violent free-surface motions and impact-loads," Computer Methods in Applied Mechanics and Engineering, vol. 200(9), pp. 1113-1125, 2011.