【Memoirs of Construction Engineering Research Institute Vol.57(papers) Nov.2015】

IMPROVED SMOOTHED PARTICLE HYDRODYNAMICS FORMULATION FOR TWO-PHASE FLOWS WITH LARGE DENSITY DIFFERENCE

Akihiko Nakayama Kong Wei Song Leong Lap Yan

ABSTRACT

The basic formulation of the smoothed particle hydrodynamics (SPH) for flows with density discontinuities such an in multi-phase flows and with a free boundary such as the upper boundary when only part of air interacting with water is calculated, has been re-examined. The form of the particle interpolation for the divergence and the pressure gradient influences the stability at the interface and at the free boundary. The improved method has been verified in the calculation of dam-break flow with air trapped under water and has been applied to an open-channel flow over steep sloped steps. Stable calculations could be done for two-phase flows with the density ratio up to 100. In the calculation of the flow over the steps, not only is the trapped air but entrained air bubbles are reproduced fairly well. The detailed variation of the time-averaged mean quantities will have to be further examined but overall prediction with relatively small number of particles is done well.

1. INTRODUCTION

The smoothed particle hydrodynamics (SPH) formulation of fluid motion was first developed for solving problems of astrophysics[1)-2)] where complex gas dynamics involving supersonic velocities with nuclear reactions is treated. It was after Monagan's demonstration[3)-4)] of its application to free surface flows that it was extended to computation of incompressible fluid. In this and much of the work following it (reviewed in Liu and Liu[5)]), an incompressible fluid is approximated by a weakly compressible fluid with sufficiently large speed of sound compared with the speed of the bulk flow. Methods that require strict incompressibility but follow the same particle interpolation technique for discretization, have also been developed. Incompressible Smoothed Particle Hydrodynamics (ISPH) method[6)-7)] and Moving Particle Semi-implicit (MPS) [8)] are such methods, in which the Poisson equation for pressure has to be solved by an iterative method and become less efficient and more elaborate. Unless strict incompressibility and accurate hydrostatic pressure distribution is required, the weak compressibility assumption proved to be efficient and practical (e.g. ref. 5)).

SPH has also been applied to incompressible fluid with varying density such as mixing of fresh and saline waters without much modifications (Monaghan and Kocharyan[9)]). It is known, however, that large density differences near the interface can cause instabilities [3)]. Valizadeh et al.[10)] suggests to modify the mass of particles near the interface to avoid the instability. The modification factors are somewhat ad hoc and more logical method is needed. Obara et al.[11)] noticed that the instability near the interface between two fluids with large density difference is caused by the large difference in the speeds of sound in the neighboring fluids, and proposed a method that makes the influence from the two fluids to be of the same order. This problem, however, occurs when two fluids are treated as physically compressible fluids. It may not solve the problems in the weakly compressible formulation of SPH in which case the speed of sound can be taken almost the same for both fluids, for example in air and water when these fluids are treated as nominally incompressible fluids. Sun et al.[12)], on the other hand, realized that in the formal derivation of the SPH equations requires that the density varies smoothly even across the interface, so that the gradient of the density is assumed to exist through the interface. They re-worked the equations without this assumption and showed that the instability problem is reduced by this treatment. However, it was only when the fluids filled the entire calculation domain without a free boundary. The formulation does not conserve the momentum and it can become unstable near the free surface of either fluids. The free surface or the boundary of fluid particles with a region without any fluid does exist if an analysis includes only small portion of the gas phase, in for example computation of air bubble entrainment and wave breaking.

In the present work, we try to find an optimum way of handling the gas-liquid interface in simulation of free-surface water flows such as in high-speed channel flow where air and water can mix near the interface. In order to save the computational load by limiting the air phase calculation to region close to the water that interacts with air. We find the momentum conserving expression for the pressure gradient terms and modify the mass by a minimal magnitude so the air-water interface with their mixing can be modeled.

The proposed method is verified in computation of collapsing water column in a closed container, and then applied to open channel flow where water and air continually flow in and flow out of the computational region. We take the flow down a stepped channel for which experimental data are available.

2. SPH METHOD FOR TWO PHASE FLOW

2.1 Basic governing equations

The SPH method expresses the spatial derivative terms in the equations of motion and the mass conservation equation using what is called the particle interpolation (e.g. refs.3),5)). If a flow quantity A such as the velocity, pressure and the density is given at a finite number of discrete points r_b called particles b, the value $A(r)$ at any point r is approximated by the following summation representation

$$A_S(\boldsymbol{r}) = \sum_b m_b \frac{A(\boldsymbol{r}_b)}{\rho_b} W(\boldsymbol{r} - \boldsymbol{r}_b, h) \tag{1}$$

where $W(\boldsymbol{r} - \boldsymbol{r}_b, h)$ is a kernel function which approximates and approaches the Dirac delta function as length h approaches zero, m_b and ρ_b are mass and the density of particle b so that the ratio m_b/ρ_b is the volume the particle b occupies. The summation approximates the integration over the volume surrounding point $\boldsymbol{r}$. From this basic particle interpolation approximation, the gradient of A can be expressed in terms of the values of the gradient of W as

$$\nabla A_S(\boldsymbol{r}) = \sum_b m_b \frac{A_b}{\rho_b} \nabla W(\boldsymbol{r} - \boldsymbol{r}_b, h) \tag{2}$$

The above formula may be used to represent the spatial derivative terms in the governing equations. Since the position $\boldsymbol{r}$ may be taken anywhere even at a moving point, it is taken at the Lagrangian point or the position of fluid particle a located at $\boldsymbol{r}_a$. The second approximation of the particle interpolation is to use the interpolant A_s in the integrands of Eqs. (1) and (2) instead of the of the original (un-interpolated) values at points $\boldsymbol{r}_b$.

$$\nabla A_a = \sum_b m_b \frac{A_b}{\rho_b} \nabla_a W_{ab} \tag{3}$$

Here the standard notation $A_a = A(\boldsymbol{r}_a)$, $\nabla_a W_{ab} = \nabla W(\boldsymbol{r}_a - \boldsymbol{r}_b)$ is used.
According to this method, the mass conservation equation

$$\frac{d\rho}{dt} = -\rho(\nabla \cdot \mathbf{v}) \tag{4}$$

written for particle a is

$$\frac{d\rho_a}{dt} = -\left[\rho(\nabla \cdot \mathbf{v})\right]_{\mathbf{r}a} = -\sum_b m_b \boldsymbol{v_b} \cdot \nabla_a W_{ab} \tag{5}$$

However, in the standard SPH as suggested by Monaghan[3], this is not used and the relation $\rho(\nabla \cdot \boldsymbol{v}) = \nabla \cdot (\rho \boldsymbol{v}) - \nabla \rho \cdot \boldsymbol{v}$ is used and the formula (3) is applied to the two terms to write

$$\frac{d\rho_a}{dt} = \sum_b m_b(\boldsymbol{v}_a - \boldsymbol{v}_b)\cdot\nabla_a W_{ab} \tag{6}$$

This relation assumes that the density varied smoothly and the gradient of ρ exists. This is the reason why Sun et al.[12] does not recommend to use it for two-phase flows with density discontinuity. However, (6) is also interpreted as adding a constant to (5) and does not necessarily require the relation of the differentiation of products. In our method we find that use of (5) cause instability at free boundaries, hence we use the symmetric form (6).

For the pressure gradient term, the form that preserves the momentum and suited for large changes of density

$$\nabla p = -\sum_b m_b\left(\frac{p_a}{\rho_a} + \frac{p_b}{\rho_b}\right)\nabla_a W_{ab} \tag{7}$$

With the Kajtar and Monaghan[13] form of viscosity the momentum equation we solve is

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b \frac{m_b}{\rho_a}\left(\frac{p_a}{\rho_a} + \frac{p_b}{\rho_b} + \Pi_{ab}\right)\nabla_a W_{ab} + \mathbf{g} \tag{8}$$

where Π_{ab} is given by the coefficients of the dynamic viscosity μ_a, μ_b and the sub-grid viscosity μ_{ta}, μ_{tb} of particles a and b

$$\Pi_{ab} = -\frac{C_\mu(\mu_a + \mu_{ta})(\mu_b + \mu_{tb})}{\rho_b(\mu_a + \mu_{ta} + \mu_b + \mu_{tb})}\frac{(\mathbf{v}_a - \mathbf{v}_b)\cdot(\mathbf{r}_a - \mathbf{r}_b)}{h\sqrt{|\mathbf{r}_a - \mathbf{r}_b|^2 + 0.01h^2}} \tag{9}$$

In the present two phase approach, the state equations for both water phase and the air phase are chosen such that the speeds of sound in both phases are the same. Therefore, the pressure of the water particles are determined by

$$p = B_w\left(\left(\frac{\rho}{\rho_{0w}}\right)^\gamma - 1\right) \tag{10}$$

and that in air by

$$p = B_a\left(\left(\frac{\rho}{\rho_{0a}}\right)^\gamma - 1\right) \tag{11}$$

where ρ_{0w} and ρ_{0a} are the initial values of the water density and the air density at rest. The coefficients B_w and B_c are taken so that the speeds of sound in water $c_w = \sqrt{\gamma B_w/\rho_{w0}}(\rho/\rho_{0w})^{\frac{\gamma-1}{2}}$ and in air $c_a = \sqrt{\gamma B_a/\rho_{a0}}(\rho/\rho_{0a})^{\frac{\gamma-1}{2}}$ for the value of γ=1/7, are about 10 times the maximum flow speeds.

The rest of the method follows out previous report (Nakayama and Hisasue[14]) and the kernel is used.

$$W_{ab}(q) = \begin{cases} \frac{1}{6}\left[(2-q)^3 - 4(1-q)^3\right], & 0 \le q \le 1, \\ \frac{1}{6}(2-q)^3 \quad , & 1 \le q \le 2, \\ 0 \quad , & q > 2 \end{cases} \tag{12}$$

so that

$$\nabla_a W_{ab} = \frac{dW_{ab}}{dq} \nabla q \tag{13}$$

is used.

2.2 Boundary conditions

As to the way the boundary conditions are imposed, we focus on how the other boundaries are treated since how the flow near solid boundary is treated has been explained as part of the sub-grid model of unresolved motion in a previous report by Nakayama and Hisasue [14].

Figure 1 shows the typical calculation region. It shows how the particles are treated in different regions. In addition to the main calculation region, it shows the wall layer near the solid boundary, inflow region at the upstream side and the outflow region at the downstream end of the main calculation region. The motion of the particles in the main calculation region are solved by the method described above. The motion of the particles in the boundary and inflow and outflow regions are not computed from the equations of motion but are set by the conditions imposed by the boundary. This is different from the common methods using boundary and/or image particles (Colagrossi and Landrini [15], Violeau and Issa [16] or Gotoh et al.[17]) or to impose an artificial repulsive force[3),5)].

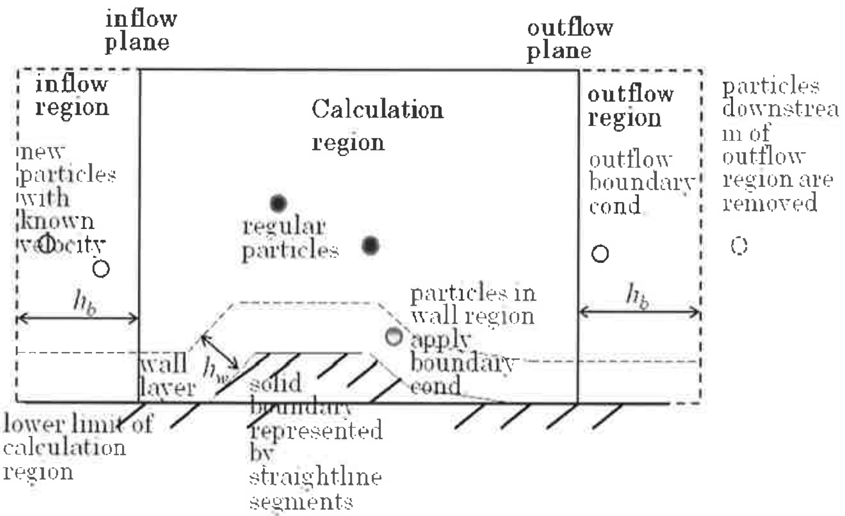

Figure 1. The boundary regions used to set boundary conditions.

For calculation of fully-developed steady flows in long channels, usually calculation in a short section is done as in many fixed-gird methods applying the 'periodic boundary condition.' In the particle method, with a link-cell method for finding the neighboring particles, we set the periodic condition on the link cells. In other words, the link cells at the most upstream are treated as the link cells neighboring the most downstream cells also and vise versa for the most downstream cells. In the application done in the following section, where the flow is periodic with the vertical shift, we shift the most upstream or most downstream cells.

3. VERIFICATION IN DAM BREAK PROBLEM

3.1 Dam break without obstacle

The above method is first tried to calculate flow within a closed container. The bench-mark case of Koshizuka et al.[18] flow with an obstacle on the floor is considered. In this case the water after striking the floor it splashes up and the air under this water is trapped between the walls and cannot escape. It is the volume not the compressibility of this air that in fluences the water surface.

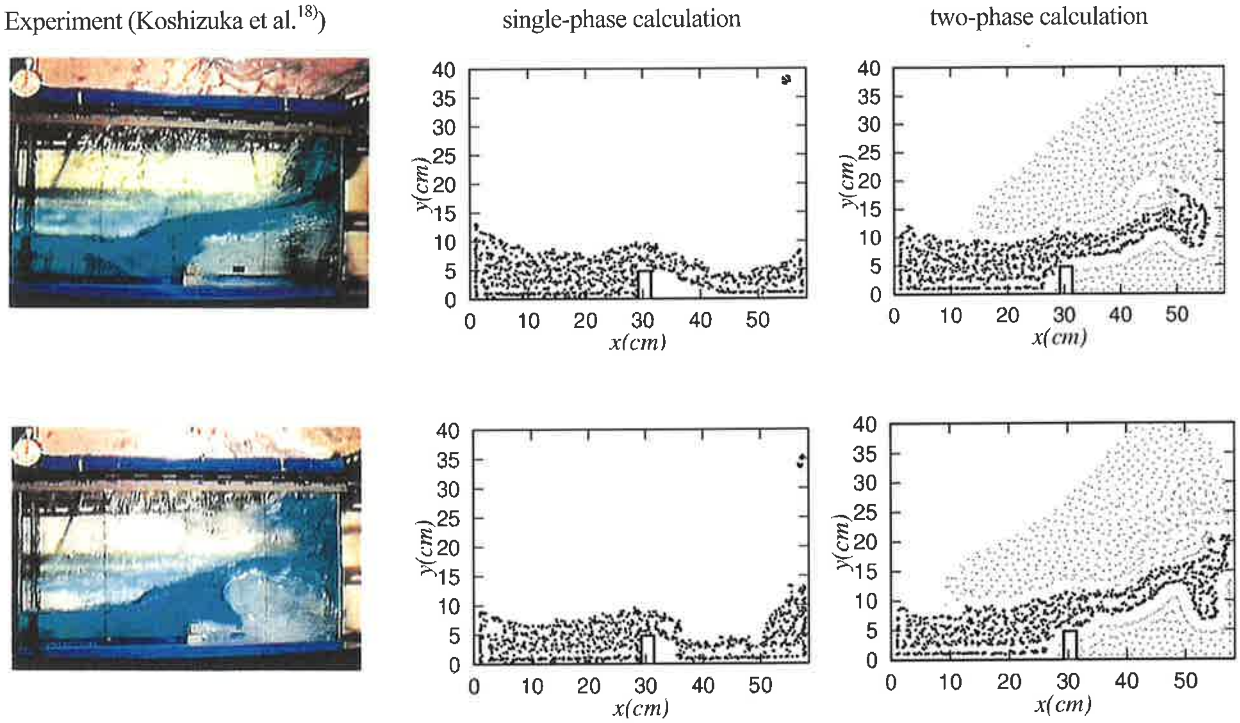

Figure 2. Two-phase flow calculation of collapsing water column in a tank. Small dots in the two-phase calculation results show are particles

Figure 2 compares the experiment, the single-phase flow calculation and the present two-phase calculation. In the two-phase-flow calculation, air particles were placed only around the initial water column and on the tank floor. This is to save the unnecessary calculation of air particles away from the water. Sun et al.'s calculation with air filling the entire tank showed that the air flow away from the water surface does not influence the water flow. For the two-phase calculation results in Figure 2, the air particles are shown in small dots while the water particles are shown in larger dots. In this flow, the air does not influence that of water except when air is trapped within water and the side walls of the tank. This is a typical case of the effects of air on the open-channel type flows. It is seen that although the air is treated as weak compressible fluid just like water, the effects of the trapped air on the water surface is reproduced well by the present method.

4. APPLICATION TO STEPPED CHANNEL FLOW

The skimming flow is a case where the water and the air can mix vigorously and the computation assuming water phase alone is difficult and not realistic. Yasuda et al.[19] has made measurement of the flow velocity and the air concentration. We will apply the present two-phase SPH method to this flow and examine the effectiveness of the proposed method.

Figure 3 is the schematic of the experiment. The flow can be classified into two distinct types shown in Figure 4. It is of interest if these different types of the flow can be simulated by the present method. We take the same bed slope θ_b as the experiment and 15.9 degs. Three cases with different depths d have been calculated. The first case is d=2.5cm, the second case d=8cm and the third case d=18cm. The first case corresponds to Type B of Yasuda et al.[19] shown in Figure 4(b). There are many (more than 6) steps in the experiment, but the flow over two steps are taken for the calculation to save the computational loads. The flow down several steps approaches a fully developed state and the calculation with a periodic boundary condition may be applied in the calculation. Therefore, for each case, the calculation was started with a column of water at rest at the top step. The inflow/outflow boundary conditions are used in these initial and intermediate flows until they flow through the calculation region. This way the air that may be trapped under the step can be simulated.

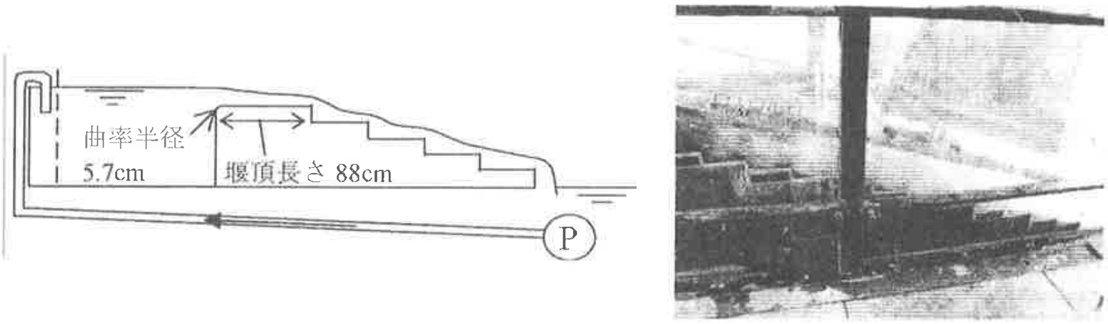

Figure 3. Flow over steps measured by Yasuda et al. [19]

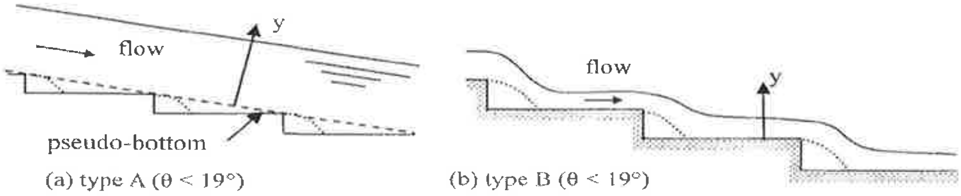

Figure 4. Two types of skimming flow over stepped channel.

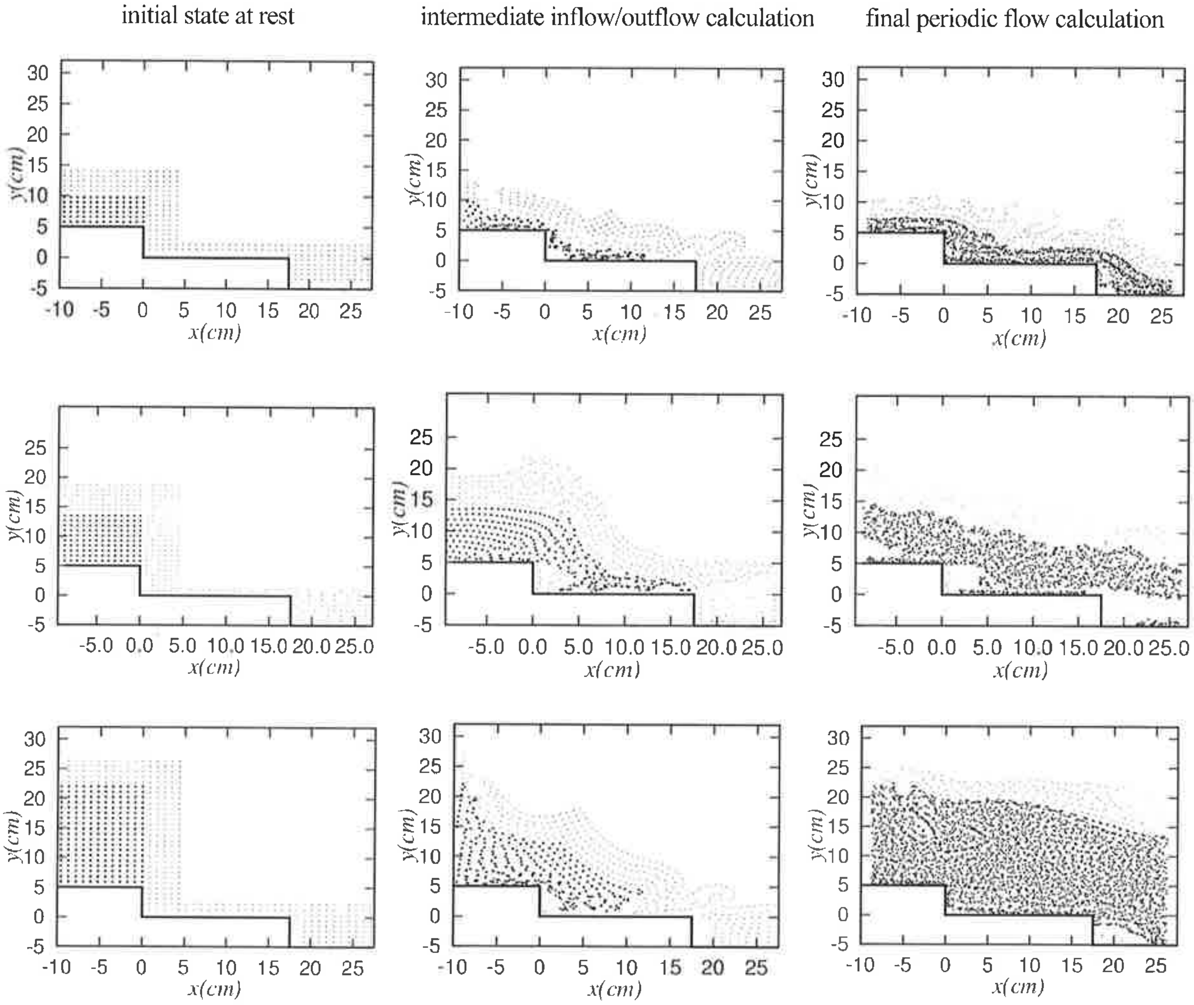

Figure 5. Three cases of the initial condition, the inflow/outflow calculation phase and periodic-flow calculation results of the flow in stepped channel.

Figure 5 shows the initial condition and the calculation results at subsequent times. It is noted that the figures include the upstream and downstream boundary regions where the boundary conditions are imposed. The water particles are shown in thick dots and the air particles are shown in small light dots. It is seen that the air trapped under the step is simulated well. However, as the intermediate flows indicate there are some difference between the flows over the two steps water flows over the steps. The final state obtained by applying the periodic boundary condition show more or less fully developed state.

The overall results appear plausible resembling the experimental observation.

Figure 6 shows the mean velocity, the mean concentration of air as implied by the mean density, and the turbulent intensities are shown for the intermediate depth case of d=18cm. These quantities are obtained by obtaining the values at the fixed positions from the values at moving particle positions using the interpolation formula, for example for the x-direction velocity u at $\boldsymbol{r}_I$

$$u(\boldsymbol{r}_I)=\sum_b m_b \frac{u_b}{\rho_b} W_{1b} \tag{14}$$

The turbulence intensity was computed by obtaining the fluctuating velocity components regardless of the phase of the particles and may be a little different from the conditioned turbulence intensity which is obtained by measuring only when the probe senses water.

The velocity distribution is seen to be more like the flow over backward-facing step with recirculation downstream of the step. In most of the flow there is no air but near the free surface and near the trapped air downstream side of the step there is a region where air and water particles are mixed. The concentration of air is large near the trapped air and near the free surface is high as observed in the experiment. The turbulence intensity is large where the flow is a mixture of air and water.

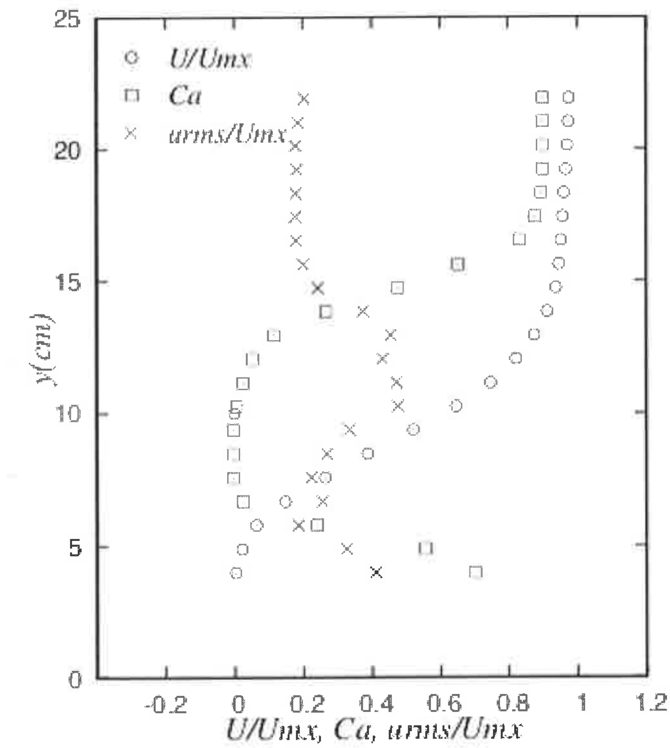

Figure 6. The mean velocity, air concentration and the turbulence intensity distribution at the center of the step.

5. CONCLUSIONS

The basic formulation of the smoothed particle hydrodynamics (SPH) has been extended to calculating flows in which gas phase fluid air interacting with liquid phase water interact near the water-air interface. Improvement has been implemented to handle the large density difference that exists near the interface that is also stable at the free boundary. The form of the particle interpolation for the divergence and the pressure gradient influences the stability at the interface and at the free boundary. This is important in simulation of air-water interaction with the calculation air motion limited to the region close to the interface for an efficient calculation.

The improved method has been verified in the calculation of dam-break flow with air trapped under water in an enclosed container. Then it has been applied to open-channel flow over steep sloped steps, where the flow comes in and goes out constantly and new particles are introduced and those leaving are deleted. Stable calculations could be achieved for two-phase flows with the density ratio up to 100. In the calculation of the flow over the steps, not only is the trapped air but entrained air bubbles are reproduced fairly well. The detailed variation of the time-averaged mean quantities will have to be further examined but overall prediction with relatively small number of particles is done well.

REFERENCES

1) Lucy, L. B., : Numerical approach to testing the fission hypothesis, *Astronomical Journal*, Vol.82, pp/1013-1024, (1977).
2) Gingold, R. A. and Monaghan, J. J., Smoothed particle hydrodynamics theory and application to non-spherical stars, *Monthly Notices of the Royal Astronomical Society*, Vol.181, pp. 375-389, (1977).
3) Monaghan, J. J.: Particle methods for hydrodynamics, *Computer Physics Reports*, Vol.3, pp. 71-124, (1985).
4) Monaghan, J. J. : Simulating free surface flows with SPH, *J. Comput. Phys.* Vol.110. pp.399-406, (1994).
5) Liu, G. R. and Liu, M. B.: *Smoothed Particle Hydrodynamics: A Meshfree Particle Method*, World Scientific Pub. Co. Inc., Singapore, (2003).
6) Cummins, S. J. and Rudman, M. : An SPH projection method, *J. Comput. Phys.* Vol.152, pp.584-607, (1999).
7) Shao, S. and Lo, E. Y. M. : Incompressible SPH method for simulating Newtonian and non-Newtonian flows with a free surface, *Advances in Water Resources*, Vol.26, No.7, pp.787-800, (2003).
8) Koshizuka, S. and Oka, Y. : Moving-Particle Semi-Implicit Method for Fragmentation of Incompressible Fluid, *Nuclear Science and Engineering*, Vol.123, pp.421-434, (1996).
9) Monaghan, J. J. and Kocharyan, A. : SPH simulation of multi-phase flow, *Computer Physics Communications*, Vol. 87 issue1-2, pp. 225-235, (1995).
10) Valizadeh, A., Shafieefar, M., Monaghan, J. J. and Salehi Neyshaboori, S.A.A. : Modeling Two-Phase Flows Using SPH Method. *Journal of Applied Sciences*, Vol.8, pp.3817-3826, (2008).
11) Obara, H., Suemura, J. and Honda, M. : Fundamental study of SPH method (1st report, treatment of 2 phase flow. Journal of Japan Society of Mechanical Engineers Series B, Vol.72 No.723, pp.78-83, (2006).
12) Sun, F, Tan M. and Xing, J.T. : Air-water two phase flow simulation using smoothed particle hydrodynamics. *International Conference on Violent Flows,* Septembet 25-27, 2012, Nantes, France, (2012).
13) Kajtar, J. and Monaghan, J. J. : SPH simulation of swimming linked bodies, *J. Comput. Phys.*, Vol. 227, pp.8568-8587, (2008).
14) Nakayama, A. and Hisasue, N. : Applicability of two-phase flow analysis based on particle method for turbulent flows, Memoirs of Construction Engineering Research Institute, Vol.55, pp.23-32, (2014).
15) Colagrossi, A. and Landrini, M. : Numerical simulation of interfacial flows by smoothed particle hydrodynamics, *J. Comput. Phys.* Vol.191, pp.448-475, (2003).
16) Violeau, D. and Issa, R. : Numerical modelling of complex turbulent free-surface flows with the SPH method: an overview, *Int. J. Numer. Meth. Fluids*, Vol. 83, pp.277-304, (2007).
17) Gotoh, H., Sibahara, T. and Sakai, T. : Sub-particle-scale turbulence model for the MPS method – Lagrangian flow model for hydraulic engineering, *Computational Fluid Dynamics Journal* Vol. 9, pp.339-347, (2001).
18) Koshizuka, S., Tamako, H. and Oka, Y. : A particle method for incompressible viscous flow with fluid fragmentation, *Computational Fluid Dynamics Journal*, Vol.4, pp.29-46, (1995).
19) Yasuda, Y., Takahashi, M. and Ohtsu, I. : Flow characteristics of skimming flow in a stepped channel, *Journal of hydraulic Engineering, JSCE*, Vol. 48, pp.499-504, (2004).

AUTHORS

Akihiko Nakayama	Ph.D., Fluid Mechanics, Hydraulics
Kong Wei Song	Student, Department of Environmental Engineering, Universiti Tunku Abdul Rahman
Leong Lap Yan	Student, Department of Environmental Engineering, Universiti Tunku Abdul Rahman