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TURBULENCE CLOSURE EFFECT ON THE FREE SURFACE PREDICTION USING MULTI-PHASE MPS METHOD

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***Abstract**: Details are given herein of the development and application of a multi-phase moving particle semi-implicit (MPS) numerical model to solve continuity and momentum equations. In the developed model, governing equations for different phases, i.e. gas, liquid and solid, were coupled in the solution procedure.*

Free surface prediction is a complicated problem which needs to be solved in many fluid flow phenomena i.e. dam break, wave breaking, etc. In recent years MPS method was widely used for non-viscous fluid flow by many researchers. Turbulence modeling issue was mainly included in these models by the means of constant eddy viscosity.

In the current study, a three dimensional multi-phase flow model using mesh less MPS method was developed to predict flow pattern. The effect of particles impact, particles interaction and turbulence are also included in the model. The model is capable of predicting particle position, velocity and pressure in each time step for both gas and liquid phases in three-dimension. In the developed model the viscous effect of the fluid was brought into account by the use of zero and two equations turbulence closure models. In this regard, Prandtl simple mixing length and standard $k-\varepsilon$ model were included to predict the free surface position in dam break type problems. Comparison of different sets of results represent a major degree of improvement from prevision studies cited in the literature, showing the importance of turbulence closure model in Lagrangian approaches. These improvement are mainly act as procedure stabilizer as well as raise the accuracy of model results.

***Keywords**: Lagrangian; Turbulence; Prandtl mixing length; $k-\varepsilon$; MPS.*

1. INTRODUCTION

In response to the needfor estimating free surface flow in many industrial and natural problems, the application of num erical methods is significantly increasing. Many investigations are performed in the field of d etermining free surf ace flow and different nu merical methods are proposed. Am ong Euler ian m ethods, the single-phase and two-p hase VOF can be nam ed. Ashigriz and Poo (1992) deve loped single-phase VOF m odel for hydrodynamics field. This model was later extended by Van der meer (1992) and resulted in SKYLLA which is a model

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based on VOF combined with an algorithm of second order accuracy. Also, the two-phase VOF model was proposed by Hieu & Tanimoto (2002). Despite the improvements of VOF method, numerical dispersion of this method seems inevitable (Van der Meer et al, 1992).

Due to the insufficient flexibility of Eulerian methods in solving problems with high deformation, moving boundary conditions and complex geometry, meshless methods are mostly used as replacement to mesh-based methods in recent years. Moving Particle Semi-implicit (MPS) is Lagrangian method. This method is basically the modified form of particle method proposed by Koshizuka and Oka (1996). In the MPS method, the fluid is divided into several moving particles and diffusion terms are calculated as these particles move. Therefore, the problem of solving diffusion terms does not occur.In particle method, the equations of continuity and momentum are converted into equations of interaction between particles in which all interactions are limited to a specific distance and weighing of interaction between two particles with distance of ris determined based on Kernel function (Atai-Ashtiani and Farhadi, 2006).The MPS model has the capability of modeling free surface of inviscid incompressible fluids and analyzing problems with high continuous interaction of fluid-structure.

However, till now MPS method has been used for modeling inviscid fluids and yet the effect of turbulence is not considered in multi-phase MPS. Also, all of the proposed models only have had the capability of estimating inviscid free surface flows. In this research, the two-phase (fluid and air) MPS method is extended for estimating free surface of viscous fluid. In the present method, the effect of turbulence is included using two turbulence models of k - ε and Prandtl's mixing length. The MPS method was used by Fayyaz and Kolahdouzan (2006) for estimating free surface of viscous fluid in which the effect of turbulence was introduced using a constant eddy viscosity. In this paper, the effect of turbulence on more accurate estimation of free surface of viscous fluid is demonstrated using Prandtl's mixing length theory and through comparing the results with those of constant viscosity. Besides, the equations of k - ε turbulence model, based on the Lagrangian method of SPH (Violeau and Issa, 2007), are introduced to MPS method successfully.

2. GOVERNING EQUATIONS

Governing equations of viscous fluid including continuity and Navier-Stokes equations are as follows (Li and Lam, 1964):

$$\begin{cases} \dfrac{1}{\rho}\dfrac{D\rho}{Dt} + \nabla.\bar{u} = 0 \\ \dfrac{D\bar{u}}{Dt} = -\dfrac{1}{\rho}\nabla\bar{p} + \upsilon_t \nabla^2 \bar{u} + f \end{cases} \tag{1}$$

where $\bar{u}$ denotes the velocity vector, t time, ρ the fluid density, p the dynamic and static pressure, υ_t the fluid eddy-viscosity, and f involves the vector of gravitational acceleration, impact force of particles and surface tension.

By adding pressure Poisson equation, the pressure term can be calculated for all particles. The Poisson equation writes as (Koshizuka and Oka, 1996):

$$\frac{\Delta\rho}{\Delta t} = -\nabla.(\Delta t\nabla p) \Rightarrow \frac{\Delta\rho}{\Delta t^2} = -\nabla^2 p \tag{2}$$

where p is the sum of static and dynamic pressures, ρ the fluid density, and t the time variable.

For considering the interaction of each particle with its neighboring particles in MPS method, the equations (1) are discretized using Laplacian, gradient and divergence operators.

To obtain a gradient vector, the operator of gradient between the particle (i) and its neighboring particles (j) is averaged using Kernel weighing function:

$$(\nabla\phi)_i = \frac{d}{n_0}\sum\frac{\phi_j-\phi_i}{\left(\left|r_j-r_i\right|^2\right)}.\left(r_j-r_i\right).w\left(\left|r_j-r_i\right|\right) \tag{3}$$

where ϕ is the calculated amount in model, d the number of dimension (for two- and three-dimensional pressures is 2 and 3, respectively), n_0 the standard density, r vector location of particle, and $w(r)$ the Kernel function. Using some modifications in gradient model, Koshizuka et al (1996) obtained more stability for this numerical method.

For determining ϕ_i in Eq. (3), they used ϕ_i' the minimum amount of ϕ between neighboring particles in the efficient radius r_e:

$$(\nabla\phi)_i = \frac{d}{n_0}\sum\frac{\phi_j-\phi_i'}{\left(\left|r_j-r_i\right|^2\right)}.\left(r_j-r_i\right).w\left(\left|r_j-r_i\right|\right)$$
$$\phi_i' = \min_{j\in J}(\phi_i,\phi_j) \qquad J=\left\{j : w\left(\left|r_j-r_i\right|\right)\neq 0\right\} \tag{4}$$

The Laplacian operator writes as:

$$\nabla^2\phi = \frac{2d}{\lambda\, n_0}\sum\left[\left(\phi_j-\phi_i\right).w\left(\left|r_j-r_i\right|\right)\right] \tag{5}$$

The presented Laplacian model is a conservative model. Because the amount separated from particle i will be attracted by particle j.

In above equations, n_i is the density of particle i in location $\vec{r}$ which defines as:

$$n_i = \sum_{i\neq j} w\left(\left|r_j-r_i\right|\right) \qquad \vec{r}_i = x\vec{i}+y\vec{j} \tag{6}$$

and the standard density n_0 is as follows:

$$n_0 = \int_V w(r)dV \tag{7}$$

and the coefficient of λ defines as:

$$\lambda = \frac{\int w(r)r^2\,dv}{\int w(r)\,dv} \tag{8}$$

In MPS method the equations of continuity and momentum are converted to interaction equations of particles using different operators. All interactions between particles are limited to a specific distance known as efficient radius. The weighing of different neighboring particles within efficient radius on the desired particle is calculated based on Kernel functions in which r is the distance between two particles i and j, and r_e is the efficient radius of Kernel function.

Since the fluid investigated in this study is viscous and the flow is turbulent, two turbulence models of Prandtl's mixing length theory and k - ε are used for determining the fluid eddy-viscosity υ_t.

The first turbulence model which provided a distribution for eddy-viscosity was provided by Prandtl (1925). In MPS method, the eddy-viscosity for each particle is obtained based on Prandtl's mixing length theory as follows:

$$\upsilon_{t,i} = k\, u_{*i}\, z_i \left(1 - \frac{z_i}{H}\right) \tag{9}$$

Also for enforcing the effect of turbulence in MPS method, the well-known k - ε equations are used.

First, for each particle such as i, a turbulence kinetic energy k_i and a energy dissipation rate ε_i are defined. Based on k - ε equations, the eddy viscosity for i particle can be writen as:

$$\upsilon_{t,i} = c_\mu \frac{k_i^2}{\varepsilon_i} \tag{10}$$

Lagrangian form of convection equation for k (turbulence kinetic energy) is as follows (Violeau and Issa, 2007):

$$\frac{dk}{dt} = P - \varepsilon + \nabla.\left[\left(\upsilon + \frac{\upsilon_t}{\sigma_k}\right)\nabla k\right] \tag{11}$$

This equation is analogous to the convection-diffusion equation where the producing term of kinetic energy P is similar to the source term, and the term of energy dissipation ε is similar to the sink term. Therefore, in the MPS method the convection equation k writes as:

$$\frac{\Delta k}{\Delta t} = P_i - \varepsilon_i + \frac{\upsilon_{k,i}\, 2d}{\lambda n_0} . \sum_{j \neq i} \left(k_j - k_i\right) . w\left(\left|r_{ij}\right|\right) \tag{12}$$

$$\upsilon_{k,i} = \upsilon + \upsilon_{t,i} / \sigma_k$$

in vector form, the source term defines as $P = -\vec{R} : \vec{S}$ where $P = -R_{ij}\, S_{ij}$ (Violeau and Issa, 2007):

$$\vec{R} = \frac{2}{3} k \vec{I} - 2\upsilon_t \vec{S} \quad , \quad P = -\vec{R} : \vec{S} \;\Rightarrow\; P = \upsilon_t S^2 \tag{13}$$

$$S = \sqrt{2\vec{S} : \vec{S}}$$

However, for preventing any overestimation of k in cases with high rates of strain variation (such as impact of water to a breakwater) it should be noted that the non-isotropic turbulence will be limited by $c_\mu^{1/2}$. Therefore, for large deformations a linear strain variation rate is considered here, and the source term of particle i limits as follows:

$$P_i = Min\left(\sqrt{c_\mu}\,, c_\mu\, S_i\, \frac{k_i}{\varepsilon_i}\right) k_i\, S_i \tag{14}$$

For estimating the rate of strain S_i one can write:

$$S_i = \frac{1}{2}\left(\frac{\partial u_i}{\partial y} + \frac{\partial v_i}{\partial x}\right) \tag{15}$$

where its MPS form is as follows:

$$S_i = \frac{d}{2\,n_0}\left(\sum_{j\neq i} \frac{u_j - u_i}{(x_j - x_i)^2 + (y_j - y_i)^2}(x_j - x_i)\, w(|r_j - r_i|) + \sum_{j\neq i} \frac{v_j - v_i}{(x_j - x_i)^2 + (y_j - y_i)^2}(y_j - y_i)\, w(|r_j - r_i|)\right) \tag{16}$$

Thus, given the S_i, k_i, ε_i and c_μ, the source term of k-ε equation can be determined. Therefore, in k-ε model the k_i can be computed using equation (12).

The energy dissipation rate ε in Lagrangian MPS form writes as equation (17):

$$\frac{d\varepsilon}{dt} = \nabla \cdot \left(\upsilon + \frac{\upsilon_t}{\sigma_\varepsilon}\nabla\varepsilon\right) + \frac{\varepsilon}{k}(C_{\varepsilon,1}P - C_{\varepsilon,2}\varepsilon)$$

$$\frac{\Delta\varepsilon}{\Delta t} = \frac{\upsilon_{\varepsilon,i}\, 2\, d}{\lambda\, n_0} \cdot \sum (\varepsilon_j - \varepsilon_i) \,.\, w(|r_{ij}|) + \frac{\varepsilon_i}{k_i}(C_{\varepsilon,1}P_i - C_{\varepsilon,2}\varepsilon_i) \tag{17}$$

$$\upsilon_{\varepsilon.i} = \upsilon + \upsilon_{t.i}/\sigma_\varepsilon$$

In this study, the constant coefficient proposed by Launder and Spaulding are used:
$c_\mu = 0.09, \sigma_k = 1.0, \sigma_\varepsilon = 1.0, C_{\varepsilon,1} = 1.44, C_{\varepsilon,2} = 1.92, \upsilon \approx 0$

3. NUMERICAL SOLUTION PROCEDURE

The Moving Particle Semi-implicit (MPS) method is used for solving the governing equations. The projection method is applied for increasing the convergence speed which separates the solution of convection and diffusion terms in Navier-Stokes equations. Hence, solution of Navier-Stokes equations will be divided into two completely different time steps. While, in first time step, the equations are solved in presence of viscosity and gravitational terms, in second time step the results obtained in the previous time step will be modified in presence of remaining terms of Navier-Stokes equations including pressure gradient, impact force of particles in two phases, surface tension force, etc.
Based on projection method, in the first time step the Navier-Stokes equations are as follows (Koshizuka and Oka, 1996):

$$\frac{D\bar{u}}{Dt} = \upsilon_t \nabla^2 \bar{u} + \bar{g} \tag{18}$$

In two-equation k - ε turbulence model the solution algorithm for each time step is as follows:
1) Determining initial k and ε at first time step;
2) Determining source term P_i of $k-\varepsilon$ equation after calculating S_i
3) Calculating turbulence kinetic energy k_i
4) Calculating coefficient of energy dissipation ε_i
5) Calculating turbulence eddy-viscosity of particle as $\upsilon_{t,i} = c_\mu \frac{k_i^{\,2}}{\varepsilon_i}$

After determining the turbulence eddy-viscosity and computing velocity variations $\nabla\bar{u}$ through solution of equations (22), the necessary corrections can be enforced on velocity and location of particles.

$$\begin{aligned} \bar{u}^* &= \Delta\bar{u}^* + \bar{u}^t \\ \bar{r}^* &= \Delta\bar{r}^* + \bar{r}^t \end{aligned} \tag{19}$$

where $\bar{u}^t$ and $\bar{r}^t$ represent velocity and location of the particle at time *t*, respectively. Also $\bar{u}^*$ and $\bar{r}^*$ are velocity and location of the particles or time * or $t+1/2$.

Given the new velocity and location of each particle, the second step of projection method will be performed through implicit solution of Poisson pressure equation and obtaining new values of pressure for each particle as follows:

$$p_i^{t+1} = \frac{\lambda n_0}{2d\sum_{i\neq j} w(|r_{ij}|)}\left[\frac{2d}{\lambda n_0}\sum_{i\neq j} p_j^{\,t}\, w(|r_{ij}|) + \frac{\rho}{\Delta t^2}\frac{n_i^{t+1}-n_0}{n_0}\right] \tag{20}$$

where *t* and *t*+1 represent the current and next time steps, respectively.

Finally, given the amount of velocity and location at time step * or $t+1/2$ and also the amount of pressure, one can enforce the correction resulted from the deviation of particle density in second phase of projection method in form of new velocities and locations for particles. This correction is enforced with solving Navier-Stokes equations. The main remaining term in Navier-Stokes equation is the pressure gradient. In the second phase of projection method the following equation is used:

$$\rho\frac{D\bar{u}}{Dt} = -\nabla p + \bar{\delta}_{gl} + \frac{\sigma k' \delta_{st}}{\rho}\bar{n} \tag{21}$$

where σ denotes the coefficient of surface tension, k' the surface curvature, $\bar{n}$ the unit surface vector perpendicular to the surface, and δ_{st} the delta function ($\delta_{st}=1$ for surface particles and $\delta_{st}=0$ for other particles). In the right-hand side of the equation (21), the second term represents the impact force between the particles of two different phases. Also, the third term represents the surface tension.

Through im plicit solution of equation (21) the am ount of velocities can be obtained. Consequently, the location of particles can be corrected so that the equations of continuity and momentum will be satisfied.

$$\bar{u}^{t+1} = \Delta\bar{u} + \bar{u}^{*}$$
$$\bar{r}^{t+1} = \Delta\bar{u}.dt + \bar{r}^{*} \tag{22}$$

4. RESULTS AND ANALYSIS

In each problem, the basic variables such as initial distance between particles (dr), time step (dt), and efficient radius (r_e) have their own optimum value based on problem conditions and Courant number. The Courant number writes as (Fayyaz and Kolahdouzan, 2008):

$$C_r = \frac{dt|u|}{dr} \leq 0.2 \tag{23}$$

In this study, the values of $dt = 0.003$, $dr = .016$ and $r_e = 1.6$ m are selected based on the computation of num erical and em pirical pro files and nature of free surface in dam breaking problems. Consequently, the dam breaking pr oblem is solv ed by MPS method and using turbulence closures such as Prandtl's mixing length theory andtwo-equation k - ε . The geometry of dam breaking problem is illustrated in Fig. (1).

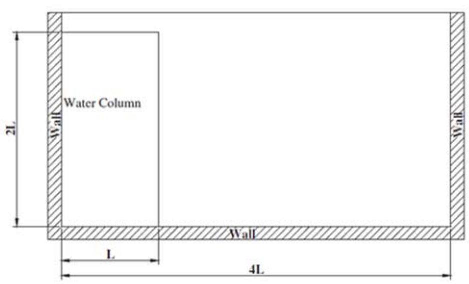
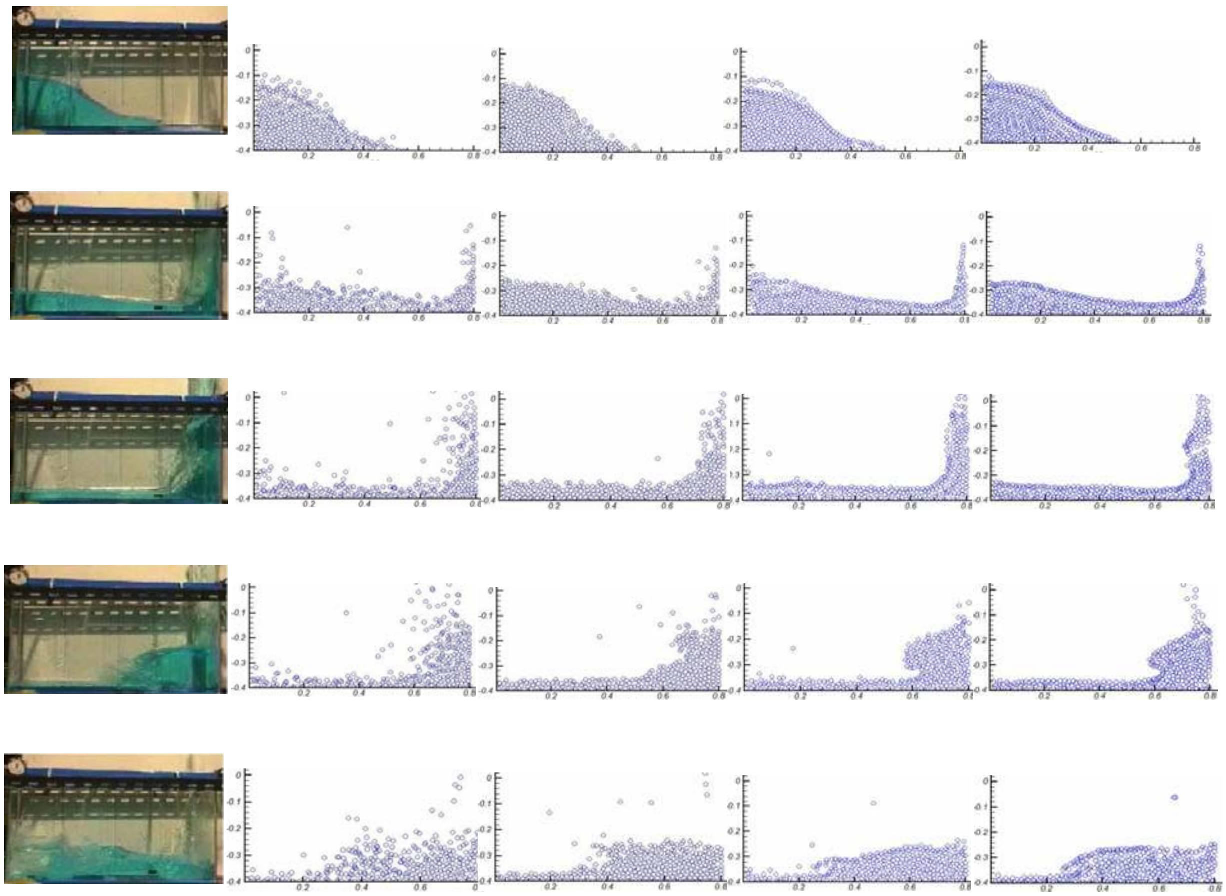


Figure 1: Geometry of dam breaking problem

The model results are compared with three sets of results of dam breaking problems in Figs (2) and (3). The first set of results is experimental data of Koshizuka (1996) which are available only for 1 second of breaking process. The second and third sets of results are numerical results of inviscid fluid and fluid with constant viscosity, respectively (Fayyaz, 2008).

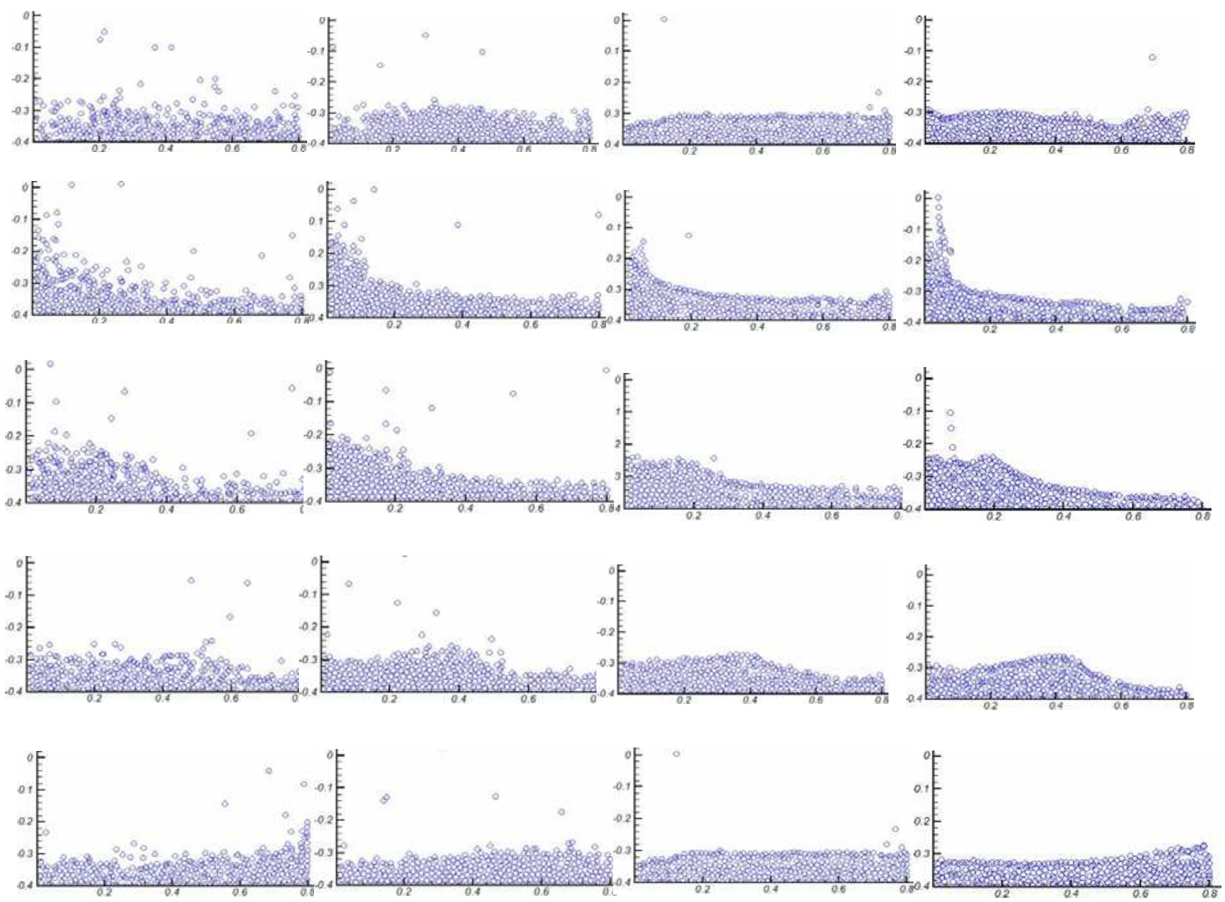
The results of comparisons indicate that using Prandtl's mixing length theory and two-equation k - ε model, the estimation of free surface flow has been improved. Moreover, a comparison is made for the number of particles in free surface flow (i.e. those with atmospheric pressure) for different time steps. The bas is of this comparison is that the less the number of free surface particles indicates better and smoother free surface flow modeling (Fig. (4)).

Comparison of thesedifferent methods reveals that using thePrandtl's mixing length theory and two-equation k - ε , the estimation of free surface flow will be improved. This improvement in accuracy of MPS method when using Prandtl's mixing length theory and k - ε turbulence closure models are due to determining the eddy-viscosity of each particle in each time step based on their location and velocity at that time step. Besides, the accuracy of model will be improved due to calculating the interaction between fluid and air phases.



(a) (b) (c) (d) (e)

Fig 2. Comparison of model results at t= 0.2, 0.4, 0.6, 0.8 and 1 S after water column collapse with results of a) Koshizuka experiments (1996) b) inviscid fluid c) fluid with constant viscosity d) Prandtl's mixing length theory e) two-equation k - ε



(a) (b) (c) (d)

Fig 3. Comparison of model results at t= 1.2, 1.4, 1.6, 1.8 and 2 S after water column collapse with results of a) inviscid fluid b) fluid with constant viscosity c) Prandtl's mixing length theory d) two-equation k - ε

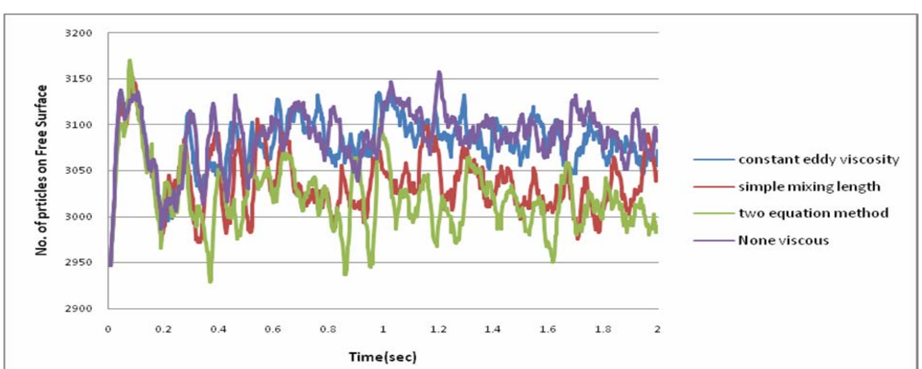


Fig 4: Results of number of free surface particles at different time steps for inviscid fluid, fluid with constant viscosity, Prandtl's mixing length theory and k - ε model

CONCLUSIONS

In this study, the effect of enforcing turbulence on estimating free surface flow is investigated using two-phase Moving Particle Semi-implicit (MPS) method. For investigating the accuracy of the developed model a dam breaking problem is solved numerically. Although the computational effort of model in case of two-phase MPS model in presence of turbulence is more than the case of inviscid fluid or fluid with constant eddy viscosity, comparison of different sets of results obtained through there methods represent the stability and accuracy of solutions in modeling complex free surface simulations. Therefore it can concluded that the stability and accuracy of two-phase MPS in modeling complex flow surfaces can be increased by considering turbulence. This can be achieved by implementing turbulence closures such as Prandtl's mixing length theory and two-equation k - ε for calculating eddy-viscosity and location at that time step. Therefore, the model is expected to be capable of modeling complex and turbulent flows such as the flow over spillways which has interaction with air.

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