A Multiphase MPS Solver for Modeling Multi-fluid Interaction with Free Surface and Its Application in Oil Spill

Guangtao Duan, Bin Chen^{*}, Ximin Zhang, Yechun Wang

State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an
710049, PR China

ABSTRACT

Numerical simulation of free surface multi-fluid flow is a challenging problem owing to the interaction between deformed interface and free surface. In this paper, a multiphase particle solver (free surface multiphase moving particle semi-implicit method, FS-MMPS) is developed to predict the early spreading flow of spilled oil where exist the oil-water interface and air-oil/air-water free surface. First, a multiphase virtual particle model is proposed to substitute the inaccurate free surface boundary condition for multiphase flow in conventional MPS methods. Specifically, virtual particles of different liquid phases are compensated outside free surface so that the pressure of free surface particles can be solved from pressure Poisson equation, thereby improving the accuracy of multi-fluid interaction at free surface. Meanwhile, a pressure gradient model based on the coupling of Taylor series expansion and dynamic specification of particle stabilizing term (PST) is proposed to simultaneously enhance accuracy and depress instability caused by multiphase virtual particles. Experiments of early spreading of thick oil slicks and continuous oil spill from a damaged tank are conducted for validation and demonstration of the accuracy and

stability enhancements in 2D. Finally, the effects of travelling wave and continuous spilling on oil spreading are investigated to show the capability of the proposed method. The spreading of thick oil slicks is accelerated when wave height increases or wave length decreases, and the largest increase of spreading rate accelerated by travelling wave is 14%.

Keywords: Moving particle semi-implicit (MPS) method; Multiphase flow; Free surface flow; Virtual particles; Pressure gradient model; Oil spills

1. Introduction

Numerical simulation of free surface multi-fluid flow is quite challenging because of the interaction between deformed interface and free surface. Oil spill is a typical example of such flow, owing to the existence of oil, water, and their interface evaluation at air-sea free surface.

Oil spills are usually serious marine disasters, which can result in tremendous economic loss and long-standing environmental damages. The early stage of spills is the best window period to clean up oil and control pollution. Predicting the early transportation behaviors of spilled oil is of great significance to the decision of emergency programs [1]. For example, *in situ* burning is an effective way to clean up thick oil slicks [2-4], and predicting the initial spreading area is of great importance to arrange containment boom in this method [2]. However, the early spreading of crude

oil is difficult to predict accurately by the simplified theoretical solutions [5-9] or experimental summaries [5, 9-11] because it is a complicated multiphase flow, influenced by manners of spilling, ship motion, wave, wind, current, etc.

In the grid-based methods for the multi-fluid interaction at free surface (e.g. oil spills), three interfaces have to be tracked/captured simultaneously and the possible topological change of interfaces has to be predicted, as shown in Fig. 1 (a). This is quite difficult for the interface algorithms, like volume of fluid (VOF) [12], level set (LS) [13] or front tracking [14] methods, because VOF and level set are not good at capturing multiple interfaces simultaneously whereas front tracking is difficult for topological change of interfaces. Therefore, few studies are devoted to the direct numerical simulations of such complex multiphase flow. In fact, grid-based methods usually treat marine oil spreading/leaking in a simplified way. Namely, the oil spilling problem was simplified as a two-phase flow by assuming free surface as a “free-slip rigid-cover” (i.e. neglecting free surface deformation) [15, 16]. For example, Zeng *et al.* [15] adopted this assumption and utilized a turbulent two-phase VOF method to simulate oil slick spreading. Gong *et al.* [16] utilized a similar method (coupling the $k-\varepsilon$ turbulence model with two-phase VOF in OpenFOAM) to simulate the leaking behaviors of oil slicks behind containment booms. However, the effects of wave or continuous spilling cannot be analyzed by these methods [15, 16] owing to the neglect of free surface deformation in the “rigid-cover” assumption.

In contrast, particle methods have great advantages in simulating such complex

flow, because air phase is usually neglected and water-air/oil-air interface can be treated as free surface [17, 18]. In particle methods, liquids are discretized into a series of Lagrangian particles, whose motion is used to represent the flow and track free surface automatically. Once oil-water interface is coupled, it will be feasible to track the motion of liquid-gas free surface and liquid-liquid interface, simultaneously. However, simulating such flows by particle methods is not easy owing to the intersection of interface with free surface. Specifically, the lack of neighbor particles makes it difficult to accurately model the multi-fluid interaction at free surface. Meanwhile, the complicated topological change (coalescence or breakup) of interface is still challenging for both grid and particle methods. Therefore, the motivation of the present paper is to develop a new particle solver to simulate the complicated multiphase flow taking place at free surface (e.g. marine oil spills).

The widely-used particle methods for fluid flow are smoothed particle hydrodynamics (SPH) [19, 20] and moving particle semi-implicit (MPS) method [21]. SPH is initially designed for astronomical problems [19, 22] and then applied to compressible/weakly-compressible flows [20], whereas the MPS method is originally developed based on the projection/semi-implicit algorithm for fully-incompressible flows [21]. Oil spilling is incompressible flow and thus the present method will be developed in the MPS framework. Another reason to choose MPS is that the pressure oscillations have been effectively alleviated owing to several remarkable improvements for the discretization of pressure Poisson equation (PPE) in MPS (see

[23-28]), which is important for oil spills since the early spreading of spilled oil is driven by pressure.

Multiphase particle methods [26, 29-41] have been developed by many researchers, but most of them are based on explicit SPH method (e.g. [29-31, 39, 40]). For semi-implicit particle methods which produce better incompressibility, the sharp density discontinuity across interface can cause instability easily. Several works (most of which are also based on ISPH) have contributed to depress this instability. For example, Hu and Adams [32] presented an extra time-step constraint to guarantee stability for multiphase ISPH method. However, this constraint will lead to exceptionally small time-step when density ratio is high. Then Hu and Adams [33] further proposed an exact-projection approach to alleviate the obstacle of extremely small time-steps, demonstrated by simulations of droplet/bubble deformation and Rayleigh-Taylor (R-T) instabilities [32, 33]. In the MPS framework, the early studies (e.g. [1, 26, 37, 42-45]) directly utilized single-phase MPS methods to simulate multiphase flows, and the interparticle properties (which are widely used in multiphase SPH [29-33] or FVM [46, 47] methods) are not adopted [38]. In this situation, the errors of multiphase simulations will increase with density ratio [38], and the quantitative verification was seldom strictly investigated. In 2012, Shakibaeinia and Jin [48] proposed a multi-viscosity model for MPS but still adopted explicit multi-density model (similar to Hu & Adams [31]) to simulate different kinds of flow instabilities (like R-T and K-H). Recently, our group developed a multiphase

moving particle semi-implicit method (MMPS) for incompressible multiphase flow and proposed two strategies (MMPS-HD and MMPS-CA) to avoid the instability caused by high density ratio. The R-T instabilities and bubble rising problems (in 2D and 3D) with a wide range of density and viscosity ratios (1000:1 and 100:1, respectively) demonstrated the reliability of the MMPS methods [38]. Thus, the present study is based on the previously-developed MMPS method.

In addition, a contoured continuum surface force (CCSF) model was proposed in our group [49] and enhanced accuracy is demonstrated for the topological change of interfaces owing to the analytical curvature calculation of smoothed color function contours. Therefore, the CCSF model will be adopted to simulate the deformation and possible coalescence/breakup of oil-water interface. In summary, the studies on semi-implicit multiphase particle methods are still focusing on developing new formulations to enhance stability and accuracy especially for flow with high density ratio. However, it is worth to note that the interface deformation takes place far from free surface in most studies above [26, 29-40, 49]. Therefore, the interaction between multi-fluid interface and free surface is seldom carefully considered before.

As to numerical simulations of oil slick spreading or leaking at free surface, there are several studies using particle methods. For example, Violeau *et al.* [50] utilized explicit SPH formulations to discretize the Reynolds-averaged Navier-Stokes (RANS) equations and firstly simulate the failure of oil containment by booms. Yang & Liu [51] also proposed an explicit multiphase SPH method with the $k-\varepsilon$ turbulence model

to investigate the effect of different factors (e.g. oil type, boom velocity, skirt angle and waves) on oil leakage from containment booms. Jeong *et al.* [1] utilized an accurate pressure gradient model and developed a high-order time integration scheme for MPS to simulate oil spills from damaged tanks. In all these studies [1, 50, 51], however, the free surface boundary condition was basically identical to single-phase flow. In other words, no special attention was paid to the interaction between interface and free surface, which is a distinguishable characteristic of oil spill flows. In this situation, the interaction among free surface particles of different phases is hardly modeled reliably, thereby decreasing the accuracy of interface deformation at free surface.

In this paper, a multiphase particle solver with special consideration on the interaction between interface and free surface will be developed based on the MMPS method [38]. First, we discuss the problem caused by the conventional arrangement of free surface boundary (i.e. assigning zero pressure to free surface particles in MMPS or MPS) in simulating oil spills. When MMPS was directly applied, the simulated oil deformation is not reliable (see Fig. 8 (b) and (f), as discussed in Section 3.1) and the spreading rate is remarkably slower than experimental measurement (see the dashed line in Fig. 9). The reason is discussed as follows. Since all the free surface particles exhibit zero pressure in original MMPS, no pressure gradient forces take place among the oil and water free surface particles. In this situation, the deformation of oil-water interface at free surface cannot be accurately simulated considering that the early

spreading of spilled oil is mainly driven by pressure gradient. Therefore, a new multiphase boundary condition for free surface is particularly necessary in MMPS to model the interaction among free surface particles of different phases effectively.

Compensating virtual particles outside free surface is an effective way to take the interaction of free surface particles into account and enhance accuracy of boundary condition [52-54]. In such methods, the pressure of virtual particles is assigned zero and that of free surface particles is solved from PPE. In this situation, pressure gradient forces take place among free surface particles and thus accuracy is improved. Recently, three parallel works [52-54] on supplementing virtual particles for MPS were reported. Chen *et al.* [52] first introduced conceptual/virtual particles into MPS and derived the modified PPE with considering the effect of virtual particles. Shibata *et al.* [53] also derived a similar PPE with considering virtual particles and proposed a corresponding pressure gradient model. Tsuruta *et al.* [54] employed potential/virtual particles to avoid the possible voids caused by strong vortex. In fact, there are two main differences among these approaches: first, virtual particles are applied to all the fluid particles when necessary by Chen *et al.* [52] and Tsuruta *et al.* [54], whereas they are only supplemented to free surface particles by Shibata *et al.* [53]; second, the positions of virtual particles are not necessary in the work of Chen *et al.* [52] and Shibata *et al.* [53], whereas they are extrapolated in Tsuruta's work [54]. However, the above approaches can only be applied to single-phase flow [52], where only one kind of virtual particles need to be supplemented. For multiphase flow, different kinds of

virtual particles should to be supplemented for multi-fluid interaction at free surface. However, few studies exist on such strategy to the best knowledge of the authors. Therefore, a multiphase virtual particle model will be proposed for MMPS in this paper so that the interaction between (oil-water) interface and free surface can be simulated more accurately.

Furthermore, the pressure gradient model has to be modified after virtual particles are introduced. Specifically, the original pressure gradient model using the minimal pressure in neighborhood [21, 55] can lead to instability easily (see detailed explanation in Section 2.4) and thus it is not adopted in the implementation of virtual particles [52-54]. Chen *et al.* [52] adopted the conservative pressure gradient model proposed by Toyota *et al.* [56] to avoid instability. Shibata *et al.* [53] derived a new general pressure gradient model for both free surface and internal particles by taking the effect of virtual particles into consideration. Tsuruta *et al.* [54] directly utilized the positions of virtual particles in their pressure gradient model. Meanwhile, pressure gradient models will affect the accuracy and stability because the early spreading of oil is mainly driven by pressure gradient force. Therefore, the performance of several pressure gradient models, including the original one proposed by Koshizuka *et al.* [21, 55], the conservative ones by Toyota *et al.* [56] and Khayyer & Gotoh [23], the first-order accurate one by Khayyer & Gotoh [25] and the general one considering virtual particles by Shibata *et al.* [53], is investigated. Based on these results, a new pressure gradient model with enhanced accuracy and stability is developed.

In summary, the paper aims to propose a multiphase virtual particle model for the multi-fluid interaction at free surface and a consistent pressure gradient model with enhanced stability and accuracy based on our previously-developed MMPS method [38]. Next, two experiments, namely initial spreading of thick oil slicks and continuous oil spills from a damaged tank, were conducted to demonstrate the improvements and validate the proposed method. Finally, the effect of wave and continuous spilling which were neglected in theoretical analyses [5-9] were discussed based on the present method. The paper is organized as follows. The numerical methods are presented in Section 2. Then the simulated results and discussions are shown in Section 3. Finally, conclusions are summarized in Section 4.

2. Numerical methods

First, the MMPS method coupled with the sub-particle scale (SPS) turbulence model proposed in our previous studies [38, 57] is briefly described. Afterwards, the free surface detection method and multiphase virtual particle model for free surface boundary condition are discussed. Finally, a pressure gradient model with enhanced accuracy and stability is developed.

2.1 Multiphase MPS method with SPS turbulence model

When the large-scale oil spills are simulated, the turbulence effect should be considered [15, 16, 50, 51]. The present study is developed in the large eddy simulation (LES) framework with consideration of the sub-particle-stress (SPS)

turbulence model [57, 58]. The Lagrangian multiphase governing equations of particle-scale flow derived by filtering the Navier-Stokes equations spatially are [38, 57, 58]:

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \bar{\mathbf{u}} = 0, \quad (1)$$

and

$$\frac{D\bar{\mathbf{u}}}{Dt} = -\frac{1}{\rho} \nabla \bar{P} + \frac{1}{\rho} \nabla \cdot (\mu \nabla \bar{\mathbf{u}}) + \frac{1}{\rho} \nabla \cdot (\rho \boldsymbol{\tau}) + \frac{\mathbf{F}_s}{\rho} + \mathbf{g}, \quad (2)$$

where $\bar{\mathbf{u}}$ and $\bar{P}$ are respectively filtered velocity and pressure; $\mathbf{g}$ is constant gravity; $\boldsymbol{\tau}$ is SPS stress; $\mathbf{F}_s$ is interface tension (between oil and water).

The SPS stress tensor ($\boldsymbol{\tau}$) represents the contribution from unresolved sub-particle scales to resolved scales and is usually modeled by the Smagorinsky model as follow:

$$\tau_{\alpha\beta} = 2\nu_t \bar{S}_{\alpha\beta} - \frac{1}{3} \delta_{\alpha\beta} \tau_{\gamma\gamma}, \quad (3)$$

$$\nu_t = (C_s \Delta)^2 (2\bar{S}_{\alpha\beta} \bar{S}_{\alpha\beta})^{1/2}, \quad (4)$$

and

$$\bar{S}_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial \bar{u}_\alpha}{\partial x_\beta} + \frac{\partial \bar{u}_\beta}{\partial x_\alpha} \right), \quad (5)$$

where ν_t is the turbulent eddy viscosity; $S_{\alpha\beta}$ is the strain rate; $\delta_{\alpha\beta}$ is the Kronecker's delta; Δ is the cutoff scale; C_s is a constant model coefficient (0.15 in present work).

In fact, the SPS stress term only contains first order derivatives and thus it can be discretized by the combination of gradient and divergence models. The detailed discretizing methods for SPS can be found in Section 2.2 of our work [57] and are not

repeated here. In the following parts, the top bar for filtered velocity ($\bar{\mathbf{u}}$) and pressure ($\bar{P}$) is omitted for convenience.

Interface tension plays an important role especially when coalescence or breakup of interfaces occurs. A contoured continuum surface force (CCSF) model has been developed in our recent work [49] and is directly adopted here as follows:

$$\left\langle \frac{\mathbf{F}_s}{\rho} \right\rangle_i = \frac{\sigma \kappa \nabla C}{\rho_i}, \quad (6)$$

where σ , κ , and C are the surface tension coefficient, local curvature, and color function, respectively. In CCSF, the local curvature κ is analytically calculated from the smoothed color function, and thus its accuracy is remarkably improved.

In the governing equations, the density ρ and viscosity μ are constant in each phase but vary sharply across interface. Here, the multi-viscosity and multi-density models are briefly described. Both the multi-viscosity and multi-density models are derived from interparticle properties in a similar way. The multi-viscosity model applying harmonic mean interparticle viscosity [38] is :

$$\langle \nabla \cdot (\mu \nabla \mathbf{u}) \rangle_i = \frac{2d}{n^0 \lambda} \sum_{j \neq i} \left\{ \frac{2\mu_i \mu_j}{\mu_i + \mu_j} (\mathbf{u}_j - \mathbf{u}_i) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}, \quad (7)$$

where i is a reference particle, j represents its neighbor particles, w is the hyperbolic weight function in MPS [21], n^0 is the constant particle number density (PND) and λ is the variance of neighbor particle distance [21, 38]. The harmonic mean interparticle viscosity produces more accurate results than the arithmetic one [38, 48] and thus the former is applied.

The above SPS stress, interface tension and multi-viscosity terms are calculated explicitly, whereas the pressure terms are solved implicitly. The multiphase pressure Poisson equation (PPE) to be solved in MMPS [38] is

$$\left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) \right\rangle_i^{k+1} = (1-\gamma) \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* - \gamma \frac{1}{\Delta t^2} \left\{ \frac{n^* - n_0}{n_0} \right\} + \alpha \frac{1}{\Delta t^2} P_i^{k+1}, \quad (8)$$

where γ is a relaxation coefficient (0.04) for the error compensation term [28], and α is an artificial compressibility coefficient (10^{-7}) [59]. Both γ and α are effective to alleviate pressure oscillations and stabilize simulations [28, 59]. The adopted divergence model in Eq. (8) is

$$\langle \nabla \cdot \mathbf{u}^* \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left\{ \frac{(\mathbf{u}_j^* - \mathbf{u}_i^*) \cdot (\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}. \quad (9)$$

The left side of the multiphase PPE (Eq. (8)) is discretized by the following multi-density model [38]:

$$\left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) \right\rangle_i^{k+1} = \frac{2d}{n_0 \lambda} \sum_{j \neq i} \left\{ \frac{2}{\rho_i + \rho_j} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}, \quad (10)$$

where the arithmetic mean interparticle density is applied for better accuracy [38].

The instability caused by density variation can be neglected due to the small density difference between oil and water.

To avoid tensile instability, the pressure gradient model which guarantees repulsive forces among particles [55] is applied:

$$\langle \nabla P \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{(P_j - P_{i,min})(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|), \quad (11)$$

where $P_{i,min}$ is the minimal pressure among neighbor particles. More details on MMPS

can be found in [38].

The free surface boundary condition in MMPS is similar to that in original MPS. However, as discussed before, the above MMPS method fails to predict the spreading of thick oil slicks reliably (see Fig. 8 (b) and (f); see detailed discussions in Section 3.1). To enhance accuracy, the virtual particle model for single-phase flow in literatures [52-54] will be extended to a multiphase one in Section 2.3. Before that, the adopted methods to accurately detect free surface particles are discussed in Section 2.2.

2.2 Detection of free surface particles

In original MPS, free surface particles are detected from the decrease of PND [21]:

$$n_i^* < \beta \cdot n^0, \quad (12)$$

where β is a coefficient (0.95). However, some internal particles may be misjudged as free surface particles by Eq. (12). Thus Tanaka & Masunaga [28] improved the detection method as follows:

$$N_i < \beta' \cdot N^0, \quad (13)$$

where N_i is the number of neighbor particles, N^0 is the initial constant one and β' is also a coefficient (0.85). More accurate detection methods based on geometrical information were also developed in literatures [53, 60-62], but they are too complicated. Tamai & Koshizuka [63] presented a method to detect the outermost layer of free surface particles. Specifically, if the following condition:

$$\begin{cases} \|\mathbf{r}_j - \mathbf{r}_i\| \geq \sqrt{2}l_0 \\ \|(\mathbf{r}_i + l_0\mathbf{n}) - \mathbf{r}_j\| < l_0 \end{cases}, \quad (14)$$

or

$$\begin{cases} \|\mathbf{r}_j - \mathbf{r}_i\| < \sqrt{2}l_0 \\ \frac{\mathbf{r}_j - \mathbf{r}_i}{\|\mathbf{r}_j - \mathbf{r}_i\|} \cdot \mathbf{n} > \frac{1}{\sqrt{2}} \end{cases}, \quad (15)$$

is satisfied, the particle will be judged as an internal particle; otherwise, the particle will be finally judged as a free surface particle. In Eqs. (14) and (15), the unit normal $\mathbf{n}$ towards outside of free surface is calculate by

$$\mathbf{n} = \frac{\mathbf{N}}{\|\mathbf{N}\|}, \quad \mathbf{N} = \frac{1}{n_i} \sum_{j \neq i} \left\{ \frac{\mathbf{r}_i - \mathbf{r}_j}{\|\mathbf{r}_j - \mathbf{r}_i\|} w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}. \quad (16)$$

In this paper, the free surface particles are detected in the following way. If Eqs. (12) and (13) are satisfied, the conditions of Eqs. (14) and (15) will be invoked to test further; otherwise, the particle is regarded as an internal liquid particle. From the above procedures, only the outermost layer of fluid particles (namely, the A-type particles in Fig. 2) are detected as free surface particles. Then, the B-type particles in Fig. 2 are detected. Specifically, B-type particles are defined as the ones whose distance from the nearest A-type particle is smaller than $\eta \times l_0$, where $\eta=2.1$ considering $r_e=3.1 \times l_0$ in this study. In this way, three layers of free surface particles are finally detected. In the following parts, the free surface particles refer to both the A-type and B-type particles. The reasons to detect free surface particles in this manner will be discussed at the end of Section 2.4.

2.3 Multiphase virtual particle model

Before developing the multiphase model, the virtual particle technique for single-phase flow is briefly described. Free surface particles face the problem of incompleteness of neighbor particles, resulting in the decrease of PND. Thus some virtual particles are added into the void neighbor area of a free surface particle as shown in Fig. 3 (a) so that the PND can rise to n^0 . Note that the virtual particles are supplemented to each free surface particle independently [53, 54]. Virtual particles are assigned to zero pressure and thus they actually replace the free surface particles in original MPS. After virtual particles are applied, the pressure of free surface particles is solved from PPE and pressure gradient interactions happen among free surface particles, thereby improving accuracy of free surface boundary. It is assumed that the PND contribution of virtual particles is $n^0 - n_i^*$, where n_i^* is the temporary PND [21]. Replacing the pressure of virtual neighbor particles by zero in PPE, one can derive modified PPE for free surface particles without referring to the positions of virtual particles (see derivation in [52-54]). In fact, the modifications happen in two places: the source term and the diagonal coefficient of the discretized PPE matrix. Considering the effect of virtual particles, a modified PND [52] is defined as follows:

$$n_i' = \max(n_i^*, n^0). \quad (17)$$

Therefore, n_i' contains the contribution of virtual particles. However, if a free surface particle is subjected to some particle clustering which does not cause n_i^* larger than n^0 , the effect of the particle clustering will not be considered in Eq.(17). This is the main

drawback of Eq.(17). Thus the following modified PND developed by Chen *et al.* [52]

is finally adopted:

$$\begin{cases} n_i' = \max(n_i^*, \tilde{n}_i) \\ \tilde{n}_i = n^0 + \sum_{j \neq i}^{N_r} \left\{ w(\|\mathbf{r}_j - \mathbf{r}_i\|) - w(l_0) \right\} \end{cases}, \quad (18)$$

where N_r is the number of real neighbor particles within a distance of l_0 from the reference particles. The modified PPE for free surface particles in single-phase flow based on n_i' [52, 53] is

$$\begin{aligned} & \frac{2d}{n_0 \lambda} \sum_{j \neq i} \left\{ (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} - \frac{2d}{n_0 \lambda} (n_i' - n_i^*) P_i^{k+1} \\ & = (1 - \gamma) \frac{\rho}{\Delta t} \nabla \cdot \mathbf{u}^* - \gamma \frac{\rho}{\Delta t^2} \left\{ \frac{n_i' - n_0}{n_0} \right\} + \alpha \frac{\rho}{\Delta t^2} P_i^{k+1} \end{aligned}, \quad (19)$$

where the coefficient of P_i^{k+1} is obviously larger than the summation of coefficients of P_j^{k+1} and the difference between them is mainly the contribution of virtual particles, which indicates the enforcement of free surface boundary condition. There are three notes for Eq. (19). First, virtual particles do not affect the divergence term because they are assumed to exhibit the same velocity with the reference particle [52, 53]. Second, n_i' is applied in the source term, which helps to prevent possible particle clustering at free surface. Lastly, Eq. (19) is only applied to free surface particles rather than all the fluid particles, which is similar to Shibata et al.'s treatment [53].

In this paper, we want to extend the above single-phase model of virtual particle implementation to a multiphase one. In the extension, the contribution of virtual particles to the source term is identical in both single-phase and multiphase simulations. However, virtual particles have complicated influence on the matrix

coefficients of multiphase PPE (Eq. (10)). In single-phase cases, specifically, the coefficients of P_i^{k+1} in Eq. (19) refer to neighbor particle j only in terms of weight function $w(\|\mathbf{r}_j - \mathbf{r}_i\|)$. In multiphase cases, however, the coefficients of P_i^{k+1} in Eq. (10) refer to particle j in terms of both weight function and inter-particle density $(\rho_i + \rho_j)/2$. That is to say, one has to determine which phase the supplemented virtual particles belong to. This is actually the main challenge in the extension. Taking the oil/water two-fluid flow as an example, one should add both virtual water and oil particles for a free surface particle, as shown in Fig. 3 (b). The numbers of supplemented virtual particles are K_w and K_o for water and oil, respectively. Considering these virtual particles, Eq. (10) for a free surface particle can be written as

$$\begin{aligned} \left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) \right\rangle_i^{k+1} &= \frac{2d}{n_0 \lambda} \sum_{j \neq i}^M \left\{ \frac{2}{\rho_i + \rho_j} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} \\ &+ \frac{2d}{n_0 \lambda} \sum_{j \neq i}^{K_o} \left\{ \frac{2}{\rho_i + \rho_o} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} \\ &+ \frac{2d}{n_0 \lambda} \sum_{j \neq i}^{K_w} \left\{ \frac{2}{\rho_i + \rho_w} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} \end{aligned} \quad , \quad (20)$$

where M is the number of real neighbor particles; ρ_o is oil density and ρ_w is water density. The pressure of virtual particles is zero in enforcing free surface boundary and thus Eq. (20) is simplified into

$$\begin{aligned} \left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) \right\rangle_i^{k+1} &= \frac{2d}{n_0 \lambda} \sum_{j \neq i}^M \left\{ \frac{2}{\rho_i + \rho_j} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} \\ &- \frac{2d}{n_0 \lambda} \left\{ \frac{2 \cdot P_i^{k+1}}{\rho_i + \rho_o} \Delta n_i^o + \frac{2 \cdot P_i^{k+1}}{\rho_i + \rho_w} \Delta n_i^w \right\} \end{aligned} \quad , \quad (21)$$

where

$$\Delta n_i^o = \sum_{j \neq i}^{K_o} w(\|\mathbf{r}_j - \mathbf{r}_i\|) \quad \text{and} \quad \Delta n_i^w = \sum_{j \neq i}^{K_w} w(\|\mathbf{r}_j - \mathbf{r}_i\|). \quad (22)$$

In Eq. (22), Δn_i^o and Δn_i^w are the PND contribution of virtual oil and water particles, respectively. Generally speaking, if there are more real water particles in the neighbor area as shown in Fig. 3 (b), more virtual water particles are expected to be supplemented. Thus we assume that the PND increase contributed by virtual particles of each phase is proportional to the PND contributed by real neighbor particles of that phase, i.e.,

$$\frac{\Delta n_i^o}{\Delta n_i^w} = \frac{n_i^o}{n_i^w}, \quad (23)$$

where n_i^o and n_i^w are the PND contributed by neighboring oil and water particles, respectively, and they satisfy

$$n_i^o + n_i^w = n_i^*. \quad (24)$$

On the other hand, the PND increase contributed by all virtual particles, $n_i' - n_i^*$, is the summation of PND increase contributed by virtual particles of each phase, i.e.,

$$\Delta n_i^o + \Delta n_i^w = n_i' - n_i^*. \quad (25)$$

Based on Eqs. (23) and (25), Δn_i^o and Δn_i^w can be determined and the results are incorporated into Eq. (21). The final revised PPE with virtual particles for multiphase flow is

$$\left\langle \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) \right\rangle_i^{k+1} = \frac{2d}{n_0 \lambda} \sum_{j \neq i}^M \left\{ \frac{2}{\rho_i + \rho_j} (P_j^{k+1} - P_i^{k+1}) w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\} - \frac{2d}{n_0 \lambda} \left\{ \frac{2 \cdot n_i^o}{\rho_i + \rho_o} + \frac{2 \cdot n_i^w}{\rho_i + \rho_w} \right\} \frac{n_i' - n_i^*}{n_i^*} P_i^{k+1}. \quad (26)$$

The above Eq. (26) can be automatically reduced to Eq. (19) if $\rho_o = \rho_w$. It is also

noted that Eq. (26) is only applied to free surface particles while internal fluid particles still utilize Eq. (10). Similar to the advantage in [52, 53], Eq. (26) does not refer to the positions of virtual particles. In addition, it is easy to extend the above two-phase virtual particle model to a multiphase case in a similar way.

2.4 Pressure gradient model with enhanced accuracy and stability

After virtual particles are added, the original pressure gradient model (e.g. Eq. (11)) cannot completely guarantee stability at free surface. The reasons are explained as follows. Eq. (11) can be decomposed into the following form:

$$\langle \nabla P \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{(P_j - P_i)(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|) + \Delta P \frac{d}{n_0} \sum_{j \neq i} \frac{(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|), \quad (27)$$

where $\Delta P = P_i - P_{i,min}$. The first part of Eq. (27) is the normal gradient model and the second error part is actually a particle stabilizing term (PST), which drives particles from dense particle region to dilute particle region. Thus PST is essential to keep particle distribution regular and further stabilize simulations in MPS (note PST is used in [1, 21, 27, 28, 45, 52, 53, 55, 64, 65]). The ΔP in Eq. (27) is called pressure difference of PST, which measures the strength of PST. It is noted that PST can only be applied to internal fluid particles because free surface particles face the incompleteness problem of neighbor particles. In original MPS, pressure of free surface particles is zero and negative pressure under free surface also has to be assigned zero to avoid instability [27]. In this situation, $P_i = P_{i,min} = 0$ (namely, $\Delta P = 0$ in Eq. (27)) for free surface particles, on which consequently PST does not work and

a collision model [65] is required for stability. However, the above strategy [27] cannot be applied to the flows where physically negative pressure happens under free surface. For example, in the simulation of continuous oil spill, some particles exhibit negative pressure near the leaking hole due to the vortices as shown in Fig. 4. If zero pressure is assigned to these particles, no pressure gradient forces takes place among these particles and thus an unphysical void emerges near the hole, as shown in Fig. 4 (a). On the other hand, after virtual particles are adopted, pressure of free surface particles is solved from PPE and they are no longer zero. In this situation, ΔP in Eq. (27) is not zero any longer and PST works on free surface particles, consequently resulting in instability. Therefore, new pressure gradient model must overcome the instabilities both at free surface and in negative pressure areas to simulate continuous oil spills.

Chen *et al.* [52] pointed out that the conservative pressure gradient model proposed by Toyota *et al.* [56],

$$\langle \nabla P \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{(P_j + P_i)(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|), \quad (28)$$

can keep simulations stable even after virtual particles are utilized. Meanwhile, Shibata *et al.* [53] derived a new pressure gradient model with the contributions of virtual particles considered:

$$\langle \nabla P \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{P_j (\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|), \quad (29)$$

which also helps to suppress the instability at free surface. Note both Eqs. (28) and

(29) can be decomposed into the form of Eq. (27) and the corresponding pressure difference of PST (i.e. ΔP) are $2P_i$ and P_i , respectively. Even though Eqs. (28) and (29) can be applied to both free surface and internal particles simultaneously, their PST strength is much larger than that of Eq. (11), since usually $2P_i > P_i > P_i - P_{i,min}$. Considering PST is essentially an artificial particle shifting technique, strong PST can benefit stability but restrict the real deformation of interface (see numerical examples in Section 3.2 and 3.3). Thus an accurate and stable pressure gradient model with appropriate PST is expected.

Another deficiency of PST in Eq. (11) or (27) is that only the minimal neighboring pressure ($P_{i,min}$) is utilized. As shown in Fig. 5 (a), when a neighboring low pressure ($P_{i,min}$) happens due to pressure oscillation, a large pressure difference of PST ($P_i - P_{i,min}$) is calculated simultaneously, which strengthen the ability of PST to keep particle uniform. In this situation, a possible instability due to pressure oscillation is avoided. On the other hand, if an unexpected high pressure $P_{i,max}$ (i.e. the largest pressure among neighbor particles) happens as shown in Fig. 5 (b), $P_i - P_{i,min}$ can just calculate an ordinary pressure difference of PST to adjust particles because $P_{i,max}$ is not referred to in Eq. (27). In this situation, the collision model [65] may be necessary to adjust particles further. Therefore, $P_{i,max} - P_{i,min}$ is a better candidate of pressure difference of PST than $P_i - P_{i,min}$ and it is better to adjust the strength of PST dynamically considering large PST can restrict the real deformation of interface.

To improve accuracy, Khayyer & Gotoh [25] proposed a corrective matrix to

modify the pressure gradient model, thereby basically guaranteeing the first-order accuracy. The corrected pressure gradient is

$$\langle \nabla P \rangle_i = \frac{1}{n_0} \sum_{j \neq i} \left\{ \frac{(P_j - P_i)(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} \mathbf{C}_i w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}, \quad (30)$$

where the non-dimensional corrective matrix $\mathbf{C}_i$ in 2D is

$$\mathbf{C}_i = \begin{pmatrix} \sum_{j \neq i} V_i \frac{w_{ij} x_{ij}^2}{r_{ij}^2} & \sum_{j \neq i} V_i \frac{w_{ij} x_{ij} y_{ij}}{r_{ij}^2} \\ \sum_{j \neq i} V_i \frac{w_{ij} y_{ij} x_{ij}}{r_{ij}^2} & \sum_{j \neq i} V_i \frac{w_{ij} y_{ij}^2}{r_{ij}^2} \end{pmatrix}^{-1}, \quad (31)$$

and

$$\begin{aligned} x_{ij} &= x_j - x_i, y_{ij} = y_j - y_i, r_{ij}^2 = x_{ij}^2 + y_{ij}^2; \\ w_{ij} &= w(r_{ij}), V_i = 1 / \sum_{j \neq i} w_{ij} \end{aligned} \quad (32)$$

However, the stability of Eq. (30) is generally not guaranteed, as pointed out by Gotoh & Khayyer [66] later. Based on above analysis, PST can also be introduced to overcome the instability problem of Eq. (30). The final pressure gradient model applying PST is:

$$\langle \nabla P \rangle_i = \frac{1}{n_0} \sum_{j \neq i} \left\{ \frac{(P_j - P_i + \xi(P_{i\max} - P_{i\min}))(\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} \mathbf{C}_i w(\|\mathbf{r}_j - \mathbf{r}_i\|) \right\}, \quad (33)$$

where ξ is a coefficient to adjust the PST strength dynamically, as discussed later.

Considering the corrective matrix $\mathbf{C}_i$ is approximately an identity matrix, it only changes the size and direction of PST slightly and thus the corrected PST is still effective to keep the particle distribution uniform. Therefore, the stability of Eq. (33) is effectively suppressed compared to Eq. (30). Meanwhile, the corrective matrix

helps to improve accuracy of Eq. (33) compared to Eqs. (27)–(29). Considering $P_{i,max}-P_{i,min}$ is roughly two times as large as $P_i-P_{i,min}$, the coefficient $\xi=0.5$ can guarantee the stability. However, we hope to adjust ξ dynamically so that the negative effects of PST can be reduced further. The following specification of ξ is found effective to keep a balance between stability and accuracy:

$$\xi = 0.2 + 2 \times \|\mathbf{N}\|, \quad (34)$$

where the vector $\mathbf{N}$ is defined by Eq. (16). The justification of Eq. (34) will be discussed in Section 3.3. When neighbor particles become irregular, a large $\|\mathbf{N}\|$ is calculated, resulting in stronger PST to keep particles uniform. When neighbor particles are basically regular, $\|\mathbf{N}\|$ is small, helping to reduce negative effects of PST. Thus Eq. (34) can dynamically adjust the strength of PST when necessary so that the accuracy of Eq. (33) is improved on the premise of guaranteeing stability. It should be noted that Eq. (34) is calibrated based present simulations and may not provide stable simulations for all kinds of problems. If instability happens, increasing the parameters can enhance stability remarkably.

As discussed before, PST cannot be applied to free surface particles and consequently neither can the improved pressure gradient model (Eq. (33)). In fact, the instability issue of the accurate gradient model (Eq. (30) or (33)) at free surface is very challenging and will not be resolved in this study. Alternatively, to overcome the instability, the less-accurate but conservative pressure gradient model (Eq. (28)) is applied to free surface particles while the improved model (Eq. (33)) is only applied

to internal particles. If free surface particles only correspond to the A-type particles in Fig. 2, some internal particles near free surface (e.g. B-type particles) will also face the incompleteness problem of neighbor particles. When Eq. (33) is applied to these internal particles, the PST can cause instability near free surface due to the incompleteness of neighbor particles. Thus three layers of free surface particles are detected in Section 2.2 to avoid the instability at free surface. Considering Eq. (33) only refers to relative difference rather than absolute value of pressure, it thus can be used to enhance stability in the area of both positive and negative pressure. In this situation, it is not necessary to change negative pressure to zero. After Eq. (33) is adopted, the void in Fig. 4 (a) is effectively avoided as shown in Fig. 4 (b). In short, Eqs (28) and (33) are respectively applied to free surface particles and internal particles to avoid the instabilities both at free surface and in negative pressure areas.

In summary, the selection of the multiphase virtual particle model and improved pressure gradient model is as follows: (a) free surface particles adopt the modified PPE (Eq. (26)) and conservative pressure gradient model (Eq. (28)); (b) internal fluid particles adopt the original PPE (Eqs. (8) and (10)) and the improved pressure gradient model (Eq. (33)). Besides, the constraints on time step are similar to those in literatures [38, 49]. For convenience, the proposed method using the multiphase virtual particles and improved pressure gradient model is named as Free Surface MMPS (FS-MMPS) in the following parts.

3. Results and Discussions

To validate the FS-MMPS method, two experiments, i.e. early spreading of thick oil slicks (Fig. 6) and continuous oil spill from a damaged tank (Fig. 7), were conducted. In the former, an oil slick with the initial thickness h is placed in the top-left corner of a reservoir, as shown in Fig. 6, where the fluid properties are also presented. Initially, oil and water are separated by a baffle, which is then removed quickly to invoke the spreading. Next, the thick oil slick deforms and spreads right. The motion of oil front is recorded by a high speed camera and then the temporal evolution of horizontal position of the oil fronts can be measured quantitatively. Three experiments with different initial thickness of oil slicks ($h = 0.04, 0.08$ and 0.12 m) were carried out to validate our FS-MMPS method. In the second experiment (Fig. 7), the oil phase with initial thickness h is stored in a damaged tank, where the hole is sealed by a baffle. After the baffle is removed, the oil continuously spills into the water in the large reservoir and spreads left. Both the motion of oil front in the large reservoir and the decline of oil surface in the right small tank are recorded quantitatively. Three experiments with different oil thickness ($h = 0.15, 0.20$ and 0.25 m) were conducted. It is note that the experiments of each working condition were repeated for three times to reduce the randomness as much as possible and that the quantitative results have good repeatability.

This section is arranged as follows. First, several numerical examples were simulated to show the improvements of multiphase virtual particle model (Section

3.1), the performance of different pressure gradient models (Section 3.2) and the effects of coefficient ξ on accuracy and stability (Section 3.3). Then the FS-MMPS method is validated by the comparisons between the simulated results and experimental observations (Section 3.4). Finally, the effects of wave and continuous spill on oil spreading are discussed briefly to show the capability of the proposed method (Section 3.5).

3.1. Accuracy of multiphase virtual particle model

The spreading of thick oil slick with $h=0.12$ m is simulated to show the accuracy of multiphase virtual particles. The “virtual particles” in this section refer to the adoption of multiphase virtual particle model (Eq. (26)) because the single-phase model cannot be directly coupled into MMPS. The initial particle distance is $l_0=1.6\times 10^{-3}$ m. The simulations with different models are conducted to show the improvements, as shown in Fig. 8 and Fig. 9. In these figures, the “original pressure gradient model” refers to Eq. (11) and the “present pressure gradient model” to Eq. (33) with ξ determined by Eq. (34). The justification of Eqs. (33) and (34) will be discussed later in Section 3.2 and 3.3, respectively. Besides, it is worth to note that the combination of “without virtual particles” and “original pressure gradient model” in Fig. 8 and Fig. 9 just represents the results directly simulated by original MMPS in Section 2.1.

First, the results predicted by original MMPS are not reliable (Fig. 8 (b), (f) and Fig. 9). At an early stage of spreading ($t = 2.0$ s), there is a gap between the top side of

oil front and the free surface, as circled in Fig. 8 (b). The reason is that no interaction happens among free surface particles whose pressure is assigned zero. In this situation, the oil-water interface has to move below rather than along free surface. At a late stage ($t = 10.0$ s), the simulated oil fronts begin to spread along free surface but the spreading rate is remarkably slower than experimental measurements. In this situation, the thick front of oil cannot be reproduced reliably either (Fig. 8 (f)). Second, when the multiphase virtual particle model is not applied, the simulated spreading behaviors are still not reliable even though the improved pressure gradient model is adopted (Fig. 8 (c), (g) and Fig. 9). The gap between the top side of interface and free surface still exists, as shown in Fig. 8 (c), and the blunt front of oil disappears in advance compared to experimental observations, as shown in Fig. 8 (g). Besides, the spreading rate is also remarkably slower than experimental result (Fig. 9). In this situation, the spreading rate is generally faster than that of original MMPS as shown in Fig. 9. In other words, accuracy is improved after the present pressure gradient model is utilized. Third, the oil distribution is basically similar to experimental observations (Fig. 8 (d) and (h)) and the quantitative agreement between simulated and experimental results is also remarkably improved (Fig. 9) after the multiphase virtual particle method is further adopted. Therefore, the multiphase virtual particles are essential to accurately predict the interaction between interface and free surface (e.g. spreading of thick oil slicks).

In summary, when virtual particles are not adopted, no interaction of pressure

gradient forces happens among free surface particles, which degrades the accuracy of interface deformation at free surface. The multiphase virtual particle model enforces multi-fluid interaction at free surface boundary and thus improves the accuracy in simulating multiphase phenomena at free surface.

3.2. Performance of different pressure gradient models

The performance of different pressure gradient models (Eqs. (27)–(29)) without using corrective matrix (Eq. (31)) is investigated based on the spreading simulations of thick oil slicks. Besides, Khayyer & Gotoh [23] also proposed a conservative pressure gradient model as follows,

$$\langle \nabla P \rangle_i = \frac{d}{n_0} \sum_{j \neq i} \frac{\left((P_j + P_i) - (P_{i,min} + P_{j,min}) \right) (\mathbf{r}_j - \mathbf{r}_i)}{\|\mathbf{r}_j - \mathbf{r}_i\|^2} w(\|\mathbf{r}_j - \mathbf{r}_i\|). \quad (35)$$

Even though its PST strength is hard to determine due to the adoption of $P_{j,min}$, its performance is also investigated. For convenience, these pressure gradient models are respectively short as PJ–PIMIN (Eq. (27) or (11)), PJ+PI (Eq. (28)), PJ (Eq. (29)) and PJ+PI–PIMIN–PJMIN (Eq. (35)). Note the PJ–PIMIN model only applies to internal fluid particles for stability. In Section 3.1, the multiphase virtual particle model is proved to be necessary in accurately simulating oil spreading and thus it is also adopted here. The initial particle distance is also $l_0 = 1.6 \times 10^{-3}$ m and the collision model [65] will be applied if particle distance is less than $0.6 \times l_0$.

The simulated snapshots of oil spreading at $t=4.0$ s are shown in Fig. 10, where the “present” model refers to the improved gradient model (Eq. (33)) with ξ

determined by Eq. (34). All the models without using corrective matrix fail to predict the thick fronts of oil slicks and their simulated oil fronts move much more slowly than the experimental observations, which can also be observed in the quantitative results as shown in Fig. 11. After the corrective matrix is adopted, the agreement between experimental results and simulated ones (presented in Fig. 10 and Fig. 11) is remarkably improved. Therefore, the corrective matrix can effectively enhance the accuracy of pressure gradient models.

Moreover, the pressure difference of PST also affects the spreading rate of oil front. As discussed in Section 2.4, the pressure difference of PST is approximately in the order of $PJ+PI > PJ > PJ-PIMIN$ for Eqs. (27)–(29). However, the spreading rate are just in the opposite order, i.e. $PJ+PI < PJ < PJ-PIMIN$, as shown in Fig. 10 and Fig. 11. Thus strong PST restricts the real deformation of interface even though it can enhance stability remarkably. When particles approach to each other, a collision model [65] is utilized to adjust and separate them artificially. The number of applying the collision model can quantitatively indicate how stable the method is. Namely, a particle method tends to be unstable when the collision number is large. The collision number in the simulations by different pressure gradient models is presented in Table 1. The $PJ+PI$ model is most stable and it does not need any particle collision to adjust particles. The PJ model requires less particle collisions than $PJ-PIMIM$ because the former has a stronger PST. These observations are consistent with the strength of PST for Eqs. (27)–(29). Thus stronger PST can enhance the stability of pressure gradient

models. When pressure oscillates, the pressure difference of PST (i.e. $P_{i,max} - P_{i,min}$) in the improved pressure gradient model (Eq. (33)) can automatically enhance the strength of PST, which is help to keep particle distribution uniform. Thus the collision number of the improve pressure gradient model is remarkably reduced, as shown in Table 1. Besides, the PJ+PI-PIMIN-PJMIN model also utilizes a high number of particle collisions as shown in Table 1, indicating it is not very stable.

From the above simulations, the corrective matrix (Eq. (31)) is essential for the accurate simulation of oil spreading; otherwise, the simulated spreading behaviors will be obviously slower than the experimental observations. Moreover, strong PST can also restrict the real deformation of interface, even though it can enhance stability. The proposed pressure gradient model with dynamic strength of PST can enhance accuracy and stability simultaneously.

3.3. Effects of coefficient ξ on accuracy and stability

In the proposed pressure gradient model (Eq. (33)), ξ is a coefficient to adjust the strength of PST. Eleven simulations with different ξ (from 0.0 to 1.0) are conducted to investigate the influence of ξ on interface deformation and stability after adopting the multiphase virtual particle model. The initial particle distance l_0 is also 1.6×10^{-3} m and the particle distance to invoke the collision model is $0.6 \times l_0$.

The simulated snapshots of thick oil slick using different ξ are presented in Fig. 12. Note the “dynamic” scheme in Fig. 12 (c) refers to Eq. (34). It can be observed that the thick fronts of oil slicks happen in all these simulations because accuracy is

improved by the corrective matrix. Moreover, oil fronts move slightly more slowly when ξ increases. The quantitative temporal evolution of oil front simulated using different ξ is shown in Fig. 13, where the solid arrows point to the direction of reducing ξ . It is clear that the larger ξ is, the more slowly the simulated oil front moves, especially when ξ is large. This is consistent the aforementioned argument that large PST can restrict the deformation of interface. On the other hand, the variation of the temporal evolution of oil front can be almost neglected when $\xi \leq 0.3$, as shown in Fig. 13. In such situations, the simulated evolution profiles are very close to the experimental observations.

On the other hand, it is not the case that the smaller ξ is, the better the simulated results are. The collision numbers in the simulations using different ξ are presented in Table 2. It is clear that the collision number increases with the decrease of ξ . That is to say particle collisions begin to play a more and more important role in stabilizing simulations with the PST strength decreased. In fact, the stabilizing effect of PST can be just partially compensated with that of particle collisions. Note that the simulation is unstable when $\xi = 0.0$ (i.e. PST is completely not utilized). Namely, the first-order accurate pressure gradient model not applying PST (i.e. Eq. (30)) cannot completely guarantee stability, which is consistent with the argument of Gotoh & Khayyer [66]. Thus the results of $\xi = 0.0$ are not presented in Fig. 12 and Fig. 13. When $\xi = 0.0$, the simulation is actually extremely unstable because a large number of particle collisions (51,869,232 times) are utilized to adjust particle distribution for stability in only 0.65s;

after that moment, the simulation finally becomes unstable. Meanwhile, considering that the pressure gradient models applying PST always produce stable results, the stability of MPS can be largely attributed to the adoption of PST. Moreover, the collision number using $\xi = 0.1$ is also obviously larger than those using $\xi = 0.2$ to 1.0 , which indicates particle collisions also play an important role in stabilizing the simulation when $\xi = 0.1$. In fact, the large number of particle collisions also has some negative influence on the interface deformation. When $\xi = 0.2$ to 0.4 , some waves can be observed behind the blunt front of oil in Fig. 12, which is consistent with the experimental observation in Fig. 10 (a). When $\xi \geq 0.5$, the formation of these waves is restricted by strong PST. On the other hand, when $\xi = 0.1$, these waves do not occur either, as shown in Fig. 12 (a), which indicates that the large number of particle collisions also restrict the formation of waves (i.e. restrict the real deformation of interface). Based on the dynamic scheme (Eq. (34)), ξ mainly varies between 0.2 and 0.4 , where these waves are successfully predicted as shown in Fig. 12. At the same time, the temporal evolution simulated by the dynamic scheme is similar to those using $\xi = 0.1$ to 0.3 , as shown in Fig. 13. Besides, the collision number using the dynamic scheme is also remarkably smaller than those using $\xi = 0.1$ to 0.3 as shown in Table 2. Thus the dynamic scheme is an appropriate approach to determine the coefficient ξ in the proposed pressure gradient model because it adjusts ξ dynamically based on the regularity of particle distribution.

In summary, large ξ can restrict the real deformation of interface due to the

strong PST. Small ξ can increase the risk of instability, thus invoking a large number of particle collisions, which can also restrict the interface deformation. The dynamic scheme (Eq. (34)) to specify ξ can keep a better balance between the accuracy of predicting interface deformation and the stability of methods. Thus the dynamic scheme is applied in the following parts.

3.4. Validation of the FS-MMPS method

In this section, both experiments of early spreading of thick oil slicks and continuous oil spill from a damaged tank are simulated to validate the proposed method.

First, the spreading of oil slick of initial thickness $h = 0.12$ m is simulated using three different particle arrangements (i.e. 468×50 ($l_0 = 3.2 \times 10^{-3}$ m), 937×100 ($l_0 = 1.6 \times 10^{-3}$ m) and 1875×200 ($l_0 = 8.0 \times 10^{-4}$ m)) to check convergence. The simulated temporal evolution of oil fronts is presented in Fig. 14 (a) and the corresponding oil distributions in Fig. 15. It can be observed that if the particle arrangement is not fine enough, the thick front of oil will fade out in advance, resulting in slow spreading rate. Basically, the particle arrangement 1875×200 is convergent and can produce reasonable results compared to experimental observations. The simulated spreading using the converged particle arrangement is compared with experimental observations in Fig. 16, where reasonable agreements can be observed. The temporal evolution of oil front in different work conditions (i.e. $h = 0.04, 0.08$ and 0.12 m) are presented in Fig. 14 (b), where the simulated results agree well with experimental measurements.

The corresponding comparisons between the simulated and experimental distributions of oil are presented in Fig. 17, where satisfactory agreements are also observed. In summary, the above qualitative and quantitative results are in good agreement with experiments.

Next, more complex flows of continuous oil spill from a damaged tank are simulated. The interface tension is employed to avoid the unphysical particle penetration through interface owing to the occurrence of strong vortices. The interface tension coefficient between oil and water is 15.2×10^{-3} N/m. First, the continuous spilling of the oil with initial thickness $h = 0.25$ m is simulated using three particle arrangement (i.e. 805×50 ($l_0 = 2 \times 10^{-3}$ m), 1610×100 ($l_0 = 1 \times 10^{-3}$ m) and 3220×200 ($l_0 = 5 \times 10^{-4}$ m)) to check convergence. As quantitatively illustrated in Fig. 18, the results of 3220×200 are similar to those of 1610×100 and thus the former is convergent. Before $t = 8.0$ s, the converged results agree well with the experimental measurements; after that moment, there are some slight difference between the simulated and experimental results. The fluctuations of spreading are caused by the sloshing waves, which is produced by the early quick spilling of oil. The processes of oil spilling simulated using the converged particle arrangement are compared with experimental observations in Fig. 19. The happening of sloshing waves is well predicted in the first three pairs of figures. Complex coalescence and break-up of water-oil interfaces are observed near the leaking hole. Generally speaking, the simulated profiles of oil are in satisfactory agreement with experimental observation.

Then the experiments in different working conditions (i.e. $h = 0.15, 0.20$ and 0.25 m) are simulated using the finest particle arrangement 3220×200 to validate the proposed method further. The comparisons between simulated and experimental quantitative results are presented in Fig. 20. Note the oil surface positions of $h = 0.20$ and 0.15 m are shifted 0.05 and 0.10 m upward in Fig. 20 (b), respectively. Basically, the simulated results agree well with the experimental measurements. The corresponding distributions of oil are shown in Fig. 21, where the secondary release of oil at $t = 4.0$ s is also well predicted. In brief, the qualitative and quantitative results predicted by the proposed method agree well with experimental observations in continuous oil spills.

In summary, the good agreements between the simulated and experimental results in different work conditions in the experiments of oil spreading and continuous spilling effectively validate the proposed FS-MMPS method.

3.5. Effects of wave and continuous spill on oil spreading

In the theoretical solutions [5-9] of oil spreading, the effects of wave and continuous release of oil are neglected for the convenience of derivation. Therefore, these effects are discussed briefly to show the capability of the proposed method in simulating complex multiphase flows at free surface.

First, the effects of travelling wave on spreading of thick oil slicks are investigated. Before the investigation, the problem of wave propagation in Lind et al.'s work [67] are simulated to show the capabilities of the present method in

predicting wave motion. The computational parameters and models are exactly the same with those in [67]. The comparison between the simulated wave shape and that by ISPH [67] is presented in Fig. 22. Meanwhile, the corresponding comparisons of pressure and velocity profiles at wave crest and trough are shown in Fig. 23. It can be observed that the present results generally agree well with those in [67]. Thus the FS-MMPS method is capable to predict wave propagation so that it can be used to investigate the effects of waves on oil spreading. The computational model to examine these effects is presented in Fig. 24, where the left side is a flap-type wavemaker to generate waves and the right side a damping area to absorb wave energy [67]. The initial thickness of simulated oil slicks is $h = 0.12$ m and the corresponding converged particle spacing $l_0 = 8.0 \times 10^{-4}$ m in the previous section is utilized. A series of simulations with different frequencies and strokes of wavemakers as shown in Table 3 are configured based on the linear wave theory [68] and simulated to separately investigate the effects of wave heights and lengths. Note that the wave heights and lengths cannot be directly specified but have to be configured by the parameters of wavemakers based on the linear wave theory. However, the errors of linear wave theory increase with the condition number α , which measures the nonlinearity of waves. Generally speaking, the linear theory cannot predict the wave properties accurately when $\alpha > 0.1$. Therefore, it is difficult to guarantee the simulated wave lengths exactly identical when the effects of wave height are examined and vice versa. In Table 3, the simulated wave heights and lengths are similar to the designed

values respectively when $\alpha < 0.1$, which also indicates that the present method is basically useful in predicting wave motion.

In Table 3, the effects of wave heights on oil spreading are investigated when the wave length is separately kept constant at 0.406, 0.813 and 1.219m as much as possible. When the designed wave length is $\lambda = 0.406$ m, the temporal evolution of oil fronts influenced by the waves of different heights are presented in Fig. 25 (a). It can be observed that after waves are considered the oil fronts spread with some fluctuations, which is similar to the effects of slosh waves in Fig. 18 and Fig. 20. The corresponding distributions of oil in waves are presented in Fig. 26. It can be observed that the average spreading velocity increases with wave heights from Fig. 25 (a), Fig. 26 and Table 3. Next, the effects of wave lengths are examined with the wave height separately kept constant at 0.0132, 0.0264 and 0.0529m as much as possible, as shown in Table 3. When the designed wave height $H=0.0529$ m, the temporal evolution of oil fronts influenced by the waves of different lengths are presented in Fig. 25 (b) and the corresponding distributions of oil in Fig. 27. It can be observed that the average spreading rate decreases with wave lengths. When Fig. 26 is compared with Fig. 27, the accelerating effect of wave lengths is less significant than that of wave heights, which can also be summarized from Table 3. In these simulations, the largest increase of spreading rate accelerated by wave is 14% with respect to that on quiescent water surface.

Second, the effects of continuous release of oil on spreading are investigated by

altering hole size, by which spilling rate is mainly determined. The adopted computational model is similar to that in Fig. 7. The hole size is altered in the following way: the top side of the hole is fixed at free surface; the bottom side is altered to obtain different hole sizes (see Fig. 29 and Fig. 30). In this situation, the spilled oil in the stable state is finally identical for all the holes of different sizes. The oil spills from the holes of six different sizes (i.e. $hole = 0.01, 0.02, 0.04, 0.06, 0.08$ and 0.10 m) are simulated. The corresponding converged particle spacing $l_0 = 5 \times 10^{-4}$ m in the previous section is utilized. The simulated temporal evolution of oil fronts and profiles of the ratios of spilled oil to all the oil are presented in Fig. 28. Note that there is a delay in the profiles of spilling ratio in Fig. 28 (b) when spilling ratio approaches 30%. The reason is that the pressure on both sides of the hole balances each other in this situation. The typical distributions of oil at an early moment ($t=1.5$ s) are presented in Fig. 29. When the hole size is large (i.e. instantaneous oil spilling), thick fronts of oil take place, resulting in high spreading velocity. When the hole size is small (i.e. continuous spilling of oil), the spilled oil exhibit high leaking velocity based on Bernoulli's principle. Therefore, the effect of hole size on spreading rate is not significant in the early stage of oil spilling ($t < 5$ s), as shown in Fig. 28 (a). However, the spilling rate of oil increases with hole size, as demonstrated in Fig. 28 (b) and Fig. 29. The typical distributions of oil at a late moment ($t=8.0$ s) are presented in Fig. 30. In the late stage of spilling ($t > 5.0$ s), the spreading rate mainly depends on the thickness of oil fronts. When the hole size is large, oil fronts are still

thick (Fig. 30) and thus the spreading rate is high (Fig. 28 (a)). However, when the hole size is small, the spilling rate is slow (Fig. 28 (b)) and the distribution of spilled oil is basically uniform (Fig. 30). The oil front is no longer thick and thus the spreading rate is slow (Fig. 28 (a)).

In summary, the spreading of thick oil slicks can be accelerated when wave height increases or wave length decreases. Moreover, the accelerating effect of wave height is more significant than wave length. In this paper, the largest increase of spreading rate accelerated by travelling wave is 14%. The continuous spilling of oil generally decreases the spreading rate because continuous spilling can change the distribution of spilled oil.

4. Conclusions

A new FS-MMPS (free surface MMPS) method is proposed for simulating multi-fluid interaction taking place at free surface. A multiphase virtual particle model is developed based on supplementing different kinds of virtual particles outside free surface and it is essential to predict the interface deformation at free surface reliably. Afterwards, a new pressure gradient model with enhanced accuracy and stability is proposed based on the coupling of corrective matrix with dynamic specification of PST. The corrective matrix can effectively improve the accuracy and the adoption of PST is essential to the stability of MPS methods. Weak PST can increase the risk of instability but strong PST can restrict real deformation of interface. The dynamic specification of PST can keep a good balance between stability and accuracy.

Two experiments, namely early spreading of thick oil slicks and continuous oil spilling from a damaged tank, are conducted for validation. The good agreements between the simulated results and experimental observations effectively validate the FS-MMPS method. Lastly, the effects of wave and continuous spilling are investigated based on the present method. The spreading of thick oil slicks is accelerated when wave height increases or wave length decreases, and the largest increase of spreading rate accelerated by travelling wave is 14% in this study. The continuous spills of oil generally decrease the spreading rate because the thick fronts of spilled oil disappear more quickly.

Acknowledgments

This research is supported by the National Science Foundation of China (51336006), the Specialized Research Fund for the Doctoral Program of Higher Education (20120201110070), and the Fundamental Research Funds for the Central Universities. Computational resources were provided by MFPE (state key laboratory of Multiphase Flow in Power Engineering) high performance computing initiative and the authors are grateful to Dr. Mingtao Li for his help in arranging the cluster.

References

- [1] S.-M. Jeong, J.-W. Nam, S.-C. Hwang, J.-C. Park, M.-H. Kim, Numerical prediction of oil amount leaked from a damaged tank using two-dimensional moving particle simulation method, *Ocean. Eng.*, 69 (2013) 70-78.
- [2] A.A. Allen, R.J. Ferek, Advantages and disadvantages of burning spilled oil, in:

- International Oil Spill Conference, American Petroleum Institute, 1993, pp. 765-772.
- [3] J.V. Mullin, M.A. Champ, Introduction/overview to in situ burning of oil spills, *Spill Science & Technology Bulletin*, 8 (2003) 323-330.
- [4] A.A. Al-Majed, A.R. Adebayo, M.E. Hossain, A sustainable approach to controlling oil spills, *J. Environ. Manag.*, 113 (2012) 213-227.
- [5] J.A. Fay, Physical processes in the spread of oil on a water surface, in: *International Oil Spill Conference*, American Petroleum Institute, 1971, pp. 463-467.
- [6] T.K. Fannelop, G.D. Waldman, Dynamics of oil slicks, *AIAA J.*, 10 (1972) 506-510.
- [7] D.P. Hoult, Oil spreading on the sea, *Annu. Rev. Fluid Mech.*, 4 (1972) 341-368.
- [8] R. Chebbi, Inertia-gravity spreading of oil on water, *Chem. Eng. Sci.*, 55 (2000) 4953-4960.
- [9] K.M. Gamzaev, Modeling the spread of an oil slick on the sea surface, *J. Appl. Mech. Tech. Ph.*, 50 (2009) 466-469.
- [10] P. Jeffery, Large-scale experiments on the spreading of oil at sea and its disappearance by natural factors, in: *International Oil Spill Conference*, American Petroleum Institute, 1973, pp. 469-474.
- [11] W. Lehr, H. Cekirge, R. Fraga, M. Belen, Empirical studies of the spreading of oil spills, *Oil and Petrochemical Pollution*, 2 (1984) 7-11.
- [12] C.W. Hirt, B.D. Nichols, Volume of fluid (VOF) method for the dynamics of free boundaries, *J. Comput. Phys.*, 39 (1981) 201-225.
- [13] M. Sussman, P. Smereka, S. Osher, A level set approach for computing solutions to incompressible two-phase flow, *J. Comput. Phys.*, 114 (1994) 146-159.
- [14] S.O. Unverdi, G. Tryggvason, A front-tracking method for viscous, incompressible, multi-fluid flows, *J. Comput. Phys.*, 100 (1992) 25-37.
- [15] L. Zeng, Z. Luo, B. Chen, Z. Yang, Z. Li, W. Lin, G. Chen, Numerical analysis of a lock-release oil slick, *Communications in Nonlinear Science and Numerical Simulation*, 15 (2010) 2222-2230.
- [16] K. Gong, P. Tkalic, H. Xu, The Numerical Investigation on Oil Slick Behavior behind the Oil Boom, *Journal of Environmental Protection*, 5 (2014) 739.
- [17] J.J. Monaghan, Simulating free surface flows with SPH, *J. Comput. Phys.*, 110 (1994) 399-406.
- [18] S. Koshizuka, Current achievements and future perspectives on particle simulation technologies for fluid dynamics and heat transfer, *J. Nucl. Sci. Technol.*, 48 (2011) 155-168.
- [19] R.A. Gingold, J.J. Monaghan, Smoothed particle hydrodynamics-theory and application to non-spherical stars, *Mon. Not. R. Astron. Soc.*, 181 (1977) 375-389.
- [20] J.J. Monaghan, Smoothed particle hydrodynamics, *Annu. rev. astron. astrophys.*, 30 (1992) 543-574.
- [21] S. Koshizuka, Y. Oka, Moving-particle semi-implicit method for fragmentation of incompressible fluid, *Nucl. Sci. Eng.*, 123 (1996) 421-434.
- [22] L.B. Lucy, A numerical approach to the testing of the fission hypothesis, *Astron.*

J., 82 (1977) 1013-1024.

- [23] A. Khayyer, H. Gotoh, Modified moving particle semi-implicit methods for the prediction of 2D wave impact pressure, *Coast. Eng.*, 56 (2009) 419-440.
- [24] A. Khayyer, H. Gotoh, A higher order Laplacian model for enhancement and stabilization of pressure calculation by the MPS method, *Appl. Ocean. Res.*, 32 (2010) 124-131.
- [25] A. Khayyer, H. Gotoh, Enhancement of stability and accuracy of the moving particle semi-implicit method, *J. Comput. Phys.*, 230 (2011) 3093-3118.
- [26] A. Khayyer, H. Gotoh, Enhancement of performance and stability of MPS mesh-free particle method for multiphase flows characterized by high density ratios, *J. Comput. Phys.*, 242 (2013) 211-233.
- [27] M. Kondo, S. Koshizuka, Improvement of stability in moving particle semi - implicit method, *Int. J. Numer. Meth. Fl.*, 65 (2011) 638-654.
- [28] M. Tanaka, T. Masunaga, Stabilization and smoothing of pressure in MPS method by quasi-compressibility, *J. Comput. Phys.*, 229 (2010) 4279-4290.
- [29] N. Grenier, M. Antuono, A. Colagrossi, D. Le Touzé, B. Alessandrini, An Hamiltonian interface SPH formulation for multi-fluid and free surface flows, *J. Comput. Phys.*, 228 (2009) 8380-8393.
- [30] N. Grenier, D. Le Touzé, A. Colagrossi, M. Antuono, G. Colicchio, Viscous bubbly flows simulation with an interface SPH model, *Ocean. Eng.*, 69 (2013) 88-102.
- [31] X. Hu, N. Adams, A multi-phase SPH method for macroscopic and mesoscopic flows, *J. Comput. Phys.*, 213 (2006) 844-861.
- [32] X. Hu, N. Adams, An incompressible multi-phase SPH method, *J. Comput. Phys.*, 227 (2007) 264-278.
- [33] X. Hu, N. Adams, A constant-density approach for incompressible multi-phase SPH, *J. Comput. Phys.*, 228 (2009) 2082-2091.
- [34] N. Tofighi, M. Yildiz, Numerical simulation of single droplet dynamics in three-phase flows using ISPH, *Comput. Math. Appl.*, 66 (2013) 525-536.
- [35] A. Zhang, P. Sun, F. Ming, An SPH modeling of bubble rising and coalescing in three dimensions, *Comput. Method. Appl. M.*, 294 (2015) 189-209.
- [36] K.S. Kim, M.H. Kim, J.-C. Park, Dynamic coupling between ship motion and three-layer-liquid separator by using moving particle simulation, *International Journal of Offshore and Polar Engineering*, 24 (2014) 122-128.
- [37] N. Shirakawa, Y. Yamamoto, H. Horie, S. Tsunoyama, Analysis of flows around a BWR spacer by the two-fluid particle interaction method, *J. Nucl. Sci. Technol.*, 39 (2002) 572-581.
- [38] G.T. Duan, B. Chen, S. Koshizuka, H. Xiang, Stable Multiphase Moving Particle Semi-implicit Method for Incompressible Interfacial Flow, *Comput. Method. Appl. M.*, 318 (2017) 636-666.
- [39] Z. Chen, Z. Zong, M. Liu, L. Zou, H. Li, C. Shu, An SPH model for multiphase flows with complex interfaces and large density differences, *J. Comput. Phys.*, 283

(2015) 169-188.

[40] K. Szewc, J. Pozorski, J.-P. Minier, Simulations of single bubbles rising through viscous liquids using smoothed particle hydrodynamics, *Int. J. Multiphase Flow*, 50 (2013) 98-105.

[41] X. Xu, J. Ouyang, T. Jiang, Q. Li, Numerical analysis of the impact of two droplets with a liquid film using an incompressible SPH method, *Journal of Engineering Mathematics*, 85 (2014) 35-53.

[42] S. Koshizuka, H. Ikeda, Y. Oka, Numerical analysis of fragmentation mechanisms in vapor explosions, *Nucl. Eng. Des.*, 189 (1999) 423-433.

[43] S. Zhang, K. Morita, N. Shirakawa, K. Fukuda, Simulation of the Rayleigh-Taylor instability with the MPS method, *Memoirs of the Faculty of Engineering. Kyushu University*, 64 (2004) 215-228.

[44] H. Gotoh, T. Sakai, Key issues in the particle method for computation of wave breaking, *Coast. Eng.*, 53 (2006) 171-179.

[45] G. Li, Y. Oka, M. Furuya, M. Kondo, Experiments and MPS analysis of stratification behavior of two immiscible fluids, *Nucl. Eng. Des.*, 265 (2013) 210-221.

[46] G. Tryggvason, R. Scardovelli, *Direct numerical simulations of gas-liquid multiphase flows*, Cambridge University Press, 2011.

[47] F. Denner, B.G. van Wachem, Fully-Coupled Balanced-Force VOF Framework for Arbitrary Meshes with Least-Squares Curvature Evaluation from Volume Fractions, *Numer. Heat. Tr. B-Fund.*, 65 (2014) 218-255.

[48] A. Shakibaeinia, Y.-C. Jin, MPS mesh-free particle method for multiphase flows, *Comput. Method. Appl. M.*, 229 (2012) 13-26.

[49] G.T. Duan, S. Koshizuka, B. Chen, A contoured continuum surface force model for particle methods, *J. Comput. Phys.*, 298 (2015) 280-304.

[50] D. Violeau, C. Buvat, K. Abed-Meraim, E. de Nanteuil, Numerical modelling of boom and oil spill with SPH, *Coast. Eng.*, 54 (2007) 895-913.

[51] X. Yang, M. Liu, Numerical modeling of oil spill containment by boom using SPH, *Sci. China. Phys. Mech. Astron.*, 56 (2013) 315-321.

[52] X. Chen, G. Xi, Z.-G. Sun, Improving stability of MPS method by a computational scheme based on conceptual particles, *Comput. Method. Appl. M.*, 278 (2014) 254-271.

[53] K. Shibata, I. Masaie, M. Kondo, K. Murotani, S. Koshizuka, Improved pressure calculation for the moving particle semi-implicit method, *Computational Particle Mechanics*, 2 (2015) 91-108.

[54] N. Tsuruta, A. Khayyer, H. Gotoh, Space potential particles to enhance the stability of projection-based particle methods, *International Journal of Computational Fluid Dynamics*, 29 (2015) 100-119.

[55] S. Koshizuka, A. Nobe, Y. Oka, Numerical analysis of breaking waves using the moving particle semi-implicit method, *Int. J. Numer. Meth. Fl.*, 26 (1998) 751-769.

[56] E. Toyota, H. Akimoto, S. Kubo, A particle method with variable spatial resolution for incompressible flows, *Proceedings of the 19th Japan Society of Fluid*

Mechanics, 9 (2005) 2.

- [57] G.T. Duan, B. Chen, Large Eddy Simulation by particle method coupled with Sub-Particle-Scale model and application to mixing layer flow, *Appl. Math. Model.*, 39 (2015) 3135-3149.
- [58] X. Xu, An improved SPH approach for simulating 3D dam-break flows with breaking waves, *Comput. Method. Appl. M.*, 311 (2016) 723-742.
- [59] H. Ikeda, S. Koshizuka, Y. Oka, H.S. Park, J. Sugimoto, Numerical analysis of jet injection behavior for fuel-coolant interaction using particle method, *J. Nucl. Sci. Technol.*, 38 (2001) 174-182.
- [60] G.A. Dilts, Moving - least - squares - particle hydrodynamics—I. Consistency and stability, *Int. J. Numer. Math. Eng.*, 44 (1999) 1115-1155.
- [61] G.A. Dilts, Moving least - squares particle hydrodynamics II: conservation and boundaries, *Int. J. Numer. Math. Eng.*, 48 (2000) 1503-1524.
- [62] C. Koh, M. Gao, C. Luo, A new particle method for simulation of incompressible free surface flow problems, *Int. J. Numer. Math. Eng.*, 89 (2012) 1582-1604.
- [63] T. Tamai, S. Koshizuka, Least squares moving particle semi-implicit method, *Computational Particle Mechanics*, (2014) 1-29.
- [64] T. Zhang, S. Koshizuka, K. Murotani, K. Shibata, E. Ishii, M. Ishikawa, Improvement of boundary conditions for non-planar boundaries represented by polygons with an initial particle arrangement technique, *International Journal of Computational Fluid Dynamics*, (2016) 1-21.
- [65] B.H. Lee, J.C. Park, M.H. Kim, S.C. Hwang, Step-by-step improvement of MPS method in simulating violent free-surface motions and impact-loads, *Comput. Method. Appl. M.*, 200 (2011) 1113-1125.
- [66] H. Gotoh, A. Khayyer, Current achievements and future perspectives for projection-based particle methods with applications in ocean engineering, *Journal of Ocean Engineering and Marine Energy*, (2016) 1-28.
- [67] S.J. Lind, R. Xu, P.K. Stansby, B.D. Rogers, Incompressible smoothed particle hydrodynamics for free-surface flows: A generalised diffusion-based algorithm for stability and validations for impulsive flows and propagating waves, *J. Comput. Phys.*, 231 (2012) 1499-1523.
- [68] D.B. Huang, *Fundamentals of Water Wave Theory* (in Chinese), National Defense Industry Press, Beijing, 2011.

Tables captions:

Table 1

The total collision times over 20 s in the oil spreading simulations using different pressure gradient models.

Table 2

The total collision times over 20 s in the oil spreading simulations using the improved pressure gradient model with different coefficient ξ .

Table 3

The parameters and simulated results in the oil spreading simulations affected by travelling waves of different wave heights and lengths.

Tables:

Table 1

The total collision times over 20 s in the oil spreading simulations using different pressure gradient models.

Model	Present	PJ-PIMIM	PJ	PJ+PI	PJ+PI-PIMIN-PJMIN
Collision times	20	12943	3853	0	687175

Table 2

The total collision times over 20 s in the oil spreading simulations using the improved pressure gradient model with different coefficient ξ .

ξ	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	Dynamic
Collision times	51869232*	15641	441	63	12	4	1	0	0	0	0	20

*51869232 for $\xi=0.0$ is the collision time just in 0.65s, after which the simulation becomes unstable.

Table 3

The parameters and simulated results in the oil spreading simulations affected by travelling waves of different wave heights and lengths.

Frequency /Hz	Stroke/m	Condition number	Wave length/m		Wave height/m		Dimensionless average spreading rate
			Designed	Simulated	Designed	Simulated	
5.851	0.031	0.050		1.221	0.0132	0.0143	0.502
	0.061	0.101	1.219	1.229	0.0264	0.0263	0.512
	0.123	0.201		1.196	0.0529	0.0601	0.550
8.000	0.020	0.060		0.821	0.0132	0.0139	0.504
	0.040	0.121	0.813	0.809	0.0264	0.0295	0.514
	0.080	0.242		0.820	0.0529	0.0615	0.556
12.223	0.011	0.104		0.411	0.0132	0.0129	0.508
	0.022	0.207	0.406	0.418	0.0264	0.0259	0.519
	0.044	0.415		0.428	0.0529	0.0469	0.573

Figures Captions:

Fig. 1. Modelling marine oil spills by different approaches.

Fig. 2. Schematic of free surface particles and virtual particles.

Fig. 3. Compensating virtual particles for a free surface particle in different cases.

Fig. 4. Snapshots of oil spilling simulations at an early moment ($t = 0.1$ s).

Fig. 5. Sketch for the unexpected (a) low pressure and (b) high pressure in the neighbor area due to pressure oscillation.

Fig. 6. The geometric parameters and fluid properties in the experiments of spreading of thick oil slicks.

Fig. 7. The geometric parameters and fluid properties in the experiments of continuous oil spill from a damaged tank.

Fig. 8. Comparison of the simulated oil distribution using different models at typical moments.

Fig. 9. Temporal evolution of oil front simulated using different models.

Fig. 10. Snapshots of oil slick spreading at $t=4.0$ s simulated using different pressure gradient models.

Fig. 11. Simulated temporal evolution of oil front using different pressure gradient models.

Fig. 12. Snapshots of oil slick spreading at $t=4.0$ s simulated using the improved pressure gradient model with different coefficient ξ .

Fig. 13. Simulated temporal evolution of oil front by the improved pressure gradient

model with different coefficient ξ .

Fig. 14. Comparisons between simulated and experimental positions of oil fronts in the experiments of oil spreading.

Fig. 15. Distributions of oil slicks simulated using different particle arrangements ($t = 7.0$ s).

Fig. 16. Comparisons between simulated and experimental distributions of oil at different moments in the spreading experiments of thick oil slicks ($h = 0.12$ m).

Fig. 17. Comparisons between simulated and experimental distributions of oil in different work conditions in the spreading experiments of thick oil slicks ($t = 2.5$ s).

Fig. 18. Convergence test in the experiments of continuous oil spills ($h = 0.25$ m).

Fig. 19. Comparisons between simulated and experimental distributions of oil at different moments in the experiments of continuous oil spills ($h = 0.25$ m).

Fig. 20. Comparisons between simulated and experimental quantitative results in different work conditions in the experiments of continuous oil spills.

Fig. 21. Comparisons between simulated and experimental distributions of oil in different work conditions in the experiments of continuous oil spills ($t = 4.0$ s).

Fig. 22. Comparison between the simulated wave propagation and that in literature [67] at $t = 9.75$ s.

Fig. 23. Comparison of mean pressure and velocity profiles between the simulated ones using the present method and those of SAWW in literature [67].

Fig. 24. Computational model for investigating effects of wave on the spreading of

thick oil slicks.

Fig. 25. Effects of travelling waves on spreading of thick oil slicks: temporal evolution of oil fronts.

Fig. 26. Snapshots of distributions of the oil slicks affected by waves of different heights (designed wave length $\lambda=0.406\text{m}$, $t=7.7\text{s}$).

Fig. 27. Snapshots of distributions of the oil slicks affected by waves of different lengths (designed wave height $H=0.0529\text{m}$, $t=7.7\text{s}$).

Fig. 28. Effects of hole sizes on spreading and spilling rates in continuous oil spills.

Fig. 29. Snapshots of distributions of oil spilled from the holes of different sizes at an early moment $t = 1.5 \text{ s}$.

Fig. 30. Snapshots of distributions of oil spilled from the holes of different sizes at a late moment $t = 8.0 \text{ s}$.

Figures:

(a) Grid methods

(b) Particle methods

Fig. 1 Modelling marine oil spills by different approaches.

Fig. 2 Schematic of free surface particles and virtual particles.

(a) Case of single phase flow

(b) Case of multiphase flow

Fig. 3 Compensating virtual particles for a free surface particle in different cases.

(a) Original pressure gradient model (Eq. (11)) with setting negative pressure to zero

(b) Present pressure gradient model (Eq. (33)) without setting negative pressure to zero

Fig. 4 Snapshots of oil spilling simulations at an early moment ($t = 0.1$ s).

Fig. 5 Sketch for the unexpected (a) low pressure and (b) high pressure in the neighbor area due to pressure oscillation.

Fig. 6 The geometric parameters and fluid properties in the experiments of spreading of thick oil slicks.

Fig. 7 The geometric parameters and fluid properties in the experiments of continuous oil spill from a damaged tank.

Fig. 8 Comparison of the simulated oil distribution using different models at typical moments.

Fig. 9 Temporal evolution of oil front simulated using different models.

Fig. 10 Snapshots of oil slick spreading at $t=4.0s$ simulated using different pressure gradient models.

Fig. 11 Simulated temporal evolution of oil front using different pressure gradient models.

Fig. 12 Snapshots of oil slick spreading at $t=4.0s$ simulated using the improved pressure gradient model with different coefficient ξ .

Fig. 13 Simulated temporal evolution of oil front by the improved pressure gradient model with different coefficient ξ .

(a) Convergence test of $h=0.12$ m

(b) Results in different work conditions

Fig. 14 Comparisons between simulated and experimental positions of oil fronts in the experiments of oil spreading.

Fig. 15 Distributions of oil slicks simulated using different particle arrangements ($t = 7.0$ s).

Fig. 16 Comparisons between simulated and experimental distributions of oil at different moments in the spreading experiments of thick oil slicks ($h = 0.12$ m).

Fig. 17 Comparisons between simulated and experimental distributions of oil in different work conditions in the spreading experiments of thick oil slicks ($t = 2.5$ s).

(a) Oil front positions in water

(b) Oil surface positions in the oil tank

Fig. 18 Convergence test in the experiments of continuous oil spills ($h = 0.25$ m).

Fig. 19 Comparisons between simulated and experimental distributions of oil at different moments in the experiments of continuous oil spills ($h = 0.25$ m).

(a) Oil front positions in water

(b) Oil surface positions in the oil tank

Fig. 20 Comparisons between simulated and experimental quantitative results in different work conditions in the experiments of continuous oil spills.

Fig. 21 Comparisons between simulated and experimental distributions of oil in different work conditions in the experiments of continuous oil spills ($t = 4.0$ s).

Fig. 22 Comparison between the simulated wave propagation and that in literature [67]
at $t = 9.75$ s.

(a) Non-hydrostatic pressure profiles

(b) Horizontal velocity profiles

Fig. 23 Comparison of mean pressure and velocity profiles between the simulated ones using the present method and those of SAWW in literature [67].

Fig. 24 Computational model for investigating effects of wave on the spreading of thick oil slicks.

(a) Wave height

(b) Wave length

Fig. 25 Effects of travelling waves on spreading of thick oil slicks: temporal evolution of oil fronts.

Fig. 26 Snapshots of distributions of the oil slicks affected by waves of different heights (designed wave length $\lambda=0.406\text{m}$, $t=7.7\text{s}$).

Fig. 27 Snapshots of distributions of the oil slicks affected by waves of different lengths (designed wave height $H=0.0529\text{m}$, $t=7.7\text{s}$).

(a) Position of oil fronts vs time

(b) Ratio of leaked oil vs time

Fig. 28 Effects of hole sizes on spreading and spilling rates in continuous oil spills.

Fig. 29 Snapshots of distributions of oil spilled from the holes of different sizes at an early moment $t = 1.5$ s.

Fig. 30 Snapshots of distributions of oil spilled from the holes of different sizes at a late moment $t = 8.0$ s.