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Surface Tension Model for Free-Surface Problems in SPH

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Abstract **–** This paper presents a surface tension model for Smoothed Particle Hydrodynamics. This model originates from previously published models based on the Continuum Surface Force approach. Its main feature is how it deals with the free surface, where particles suffer from particle deficiency. The model is tested in two dimensions using oscillating and static cylindrical rod problems. Its sensitivity to spatial resolution was evaluated, and some of the model's features discovered. Overall, the model seems to provide accuracy sufficient for most practical applications.

Keywords**:** SPH, Surface tension, Free-surface, CFD

1. Introduction

Surface tension is a phenomenon occurring on interfaces between immiscible phases, usually liquid and gas or two liquids. Molecules of liquids posse more energy when they are close to the surface than if they are surrounded by the same phase from all sides. As a result, liquids tend to have as small surface as possible. This fact influences fluid's behavior noticeably, especially in small scale problems like droplet interactions, where surface forces are comparable to inertial and viscous forces.

In continuum mechanics, surface tension is described by the Young-Laplace equation

$$\Delta p = -\sigma \nabla \cdot \hat{\mathbf{n}} \tag{1}$$

which states that pressure step on the interface Δp is directly proportional to surface tension coefficient σ and divergence of the unit surface normal $\hat{\mathbf{n}}$. This divergence represents the mean curvature of the surface.

One of the ways how to implement this equation into numerical methods is Continuum Surface Force (CSF), first introduced by Brackbill et al. [1] for the use in Finite Volumes Method (FVM), where the pressure step on the interface is caused by a force exerted on fluid volume near the interface. This concept proved itself to be viable for SPH as well, and Morris [2] or Hu and Adams [3] presented such methods for multiphase flows. Some surface tension models for free-surface flows, where the lighter gaseous phase is completely omitted, have been published as well by Zhang [4] or Ordoubadi et al. [5]. These works present more complicated ways of interface tracking than in a proper multiphase flow.

This work aims to show a possible way of modeling surface tension in free-surface flows without too complicated algorithms but reasonable robustness and accuracy at the same time. The proposed method is described in detail and its abilities are presented on simple two-dimensional problems. The results are compared with exact solutions, and the results are discussed.

2. Computational Method

Smoothed Particle Hydrodynamics (SPH) is a particle computational method for solving partial differential equations. Its Lagrangian nature makes it particularly suitable for solutions of transient, multiphase problems in hydrodynamics. In this work, weakly compressible SPH is employed, which is a way of solving incompressible fluid flow as a slightly compressible one. More information about the method can be found, for example, in the monograph by Liu and Liu [6].

2.1. Governing Equations

The governing equations of fluid motion are the continuity equation and the momentum equation. In SPH form with Lagrangian time derivatives these can be written as

$$\frac{\mathrm{D}\rho_i}{\mathrm{D}t} = \rho_i \sum_j \frac{m_j}{\rho_j} \left(\mathbf{v}_i - \mathbf{v}_j\right) \cdot \nabla W_{ij} \tag{2}$$

$$\frac{\mathrm{D}\mathbf{v}_i}{\mathrm{D}t} = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij}\right) \nabla W_{ij} + \mathbf{a}_i \tag{3}$$

where t is time, ρ is density, m mass, and $\mathbf{v}$ velocity. Subscripts i and j indicate particles. Function W is a so-called weight function, and in this case, the truncated Gaussian kernel was used [6]. It can be described by the relation

$$W_{ij}(R,h) = \begin{cases} \pi^{-d/2} h^{-d} \exp(-R^2) & \text{if } R \leq 3 \\ 0 & \text{if } R > 3 \end{cases} \tag{4}$$

where d is number of spatial dimensions, h is so-called smoothing length, which is a parameter related to spatial resolution, and $R = \left|\mathbf{x}_i - \mathbf{x}_j\right|/h$ is normalized particle distance. Vector $\mathbf{x}$ denotes spatial position. Term Π is the numerical viscosity term serving mostly for numerical stabilization [7]. It is defined as

$$\Pi_{ij} = \max\left[-\frac{\alpha c_{ij} h_{ij}}{\varrho_{ij}} \frac{\left(\mathbf{v}_i - \mathbf{v}_j\right) \cdot \left(\mathbf{x}_i - \mathbf{x}_j\right)}{\left(\mathbf{x}_i - \mathbf{x}_j\right) \cdot \left(\mathbf{x}_i - \mathbf{x}_j\right) + \varepsilon h_{ij}^2}; 0\right] \tag{5}$$

where α is the artificial viscosity coefficient and c is speed of sound (physical or numerical). Mean values of the particle pair is taken for the variables with index ij. Parameter $\varepsilon = 0.01$ serves for avoiding division by zero. Term $\mathbf{a}$ is the external acceleration caused by surface tension, which is described in detail in subsection 2.2.

An equation of state has to be used to close the system of equations (2) and (3). The equation

$$p = \frac{c^2 \rho_0}{\gamma} \left[\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right] \tag{6}$$

first used by Monaghan [8] is employed. Parameter $\gamma = 7$, ρ_0 is reference density, and c is numerical speed of sound. It is chosen according to particular problem to reach small changes in density, preferably no more than 1%.

2.2. Surface Tension Model

The Young-Laplace equation (1) has to be transformed into a form suitable for SPH. The form presented in the following paragraphs originates from the first method published by Morris [2]. For the location of an interface serves so-called color function f. Since there is only one phase in free-surface problems, for all particles holds $f_i = 1$. However, this function is not suitable for finding surface normal. First, it has to be smoothed near the interface. A modified colour function f^* is obtained using the formula

$$f_i^* = \sum_j \frac{m_j}{\rho_j} f_j W_{ij} \tag{7}$$

In proper multiphase problems, f^* goes down from unity in respective phase to zero outside this phase. But in free surface problems, it cannot reach zero, since there are no particles of another phase. To fix this, f^* is transformed to f^{**} using relation

$$f_i^{**} = (af_i^* - a + 1)^b \tag{8}$$

The further presented results were computed for $a = 2$ and $b = 4$. Other functions can be used for this transformation as well.

Surface normal vector $\mathbf{n}$ is now found as gradient of color function f^{**} using formula

$$\mathbf{n}_i = \sum_j \frac{m_j}{\rho_j} \left(f_j^{**} - f_i^{**}\right) \nabla W_{ij} \tag{9}$$

To exclude spurious normal vectors from further computations, they are evaluated by their magnitude. This is practically done by a sorting function N defined as

$$\mathrm{N}_i = \begin{cases} 1 \text{ if } |\mathbf{n}_i| \geq 0.01/h_i \\ 0 \text{ if } |\mathbf{n}_i| < 0.01/h_i \end{cases} \tag{10}$$

A correction function C is defined

$$C_i = \sum_j \frac{m_j}{\rho_j} \min\left(\mathrm{N}_i, \mathrm{N}_j\right) W_{ij} \tag{11}$$

and the corrected normal vectors $\mathbf{n}^*$ are computed as

$$\mathbf{n}_i^* = \mathbf{n}_i / C_i \tag{12}$$

The divergence of unit normal vector is calculated using formula including correction

$$(\nabla \cdot \hat{\mathbf{n}}_i) = \sum_j \min\left(\mathrm{N}_i, \mathrm{N}_j\right) \frac{m_j}{\rho_j} \left(\hat{\mathbf{n}}_j - \hat{\mathbf{n}}_i\right) \nabla W_{ij} / C_i \tag{13}$$

This divergence is then averaged to smooth out the curvature field and eliminate extreme values that lead to surface disruptions

$$(\nabla \cdot \hat{\mathbf{n}}_i)^* = \sum_j \frac{m_j}{\rho_j} (\nabla \cdot \hat{\mathbf{n}}_i) W_{ij} / C_i \tag{14}$$

The final surface tension acceleration vector in equation (3) stands

$$\mathbf{a}_i = -\frac{\sigma}{\rho_i} (\nabla \cdot \hat{\mathbf{n}}_i)^* \mathbf{n}_i^* \tag{15}$$

4. Test Problem Definition

The surface tension model was tested on a two-dimensional oscillating rod. This problem can show its ability in both static and dynamic behavior. The theoretical solution of the problem is known, so the precision of the method can be evaluated as well.

Initially, identical fluid particles arranged into regular triangular lattice form an ellipse: a two-dimensional representation of an elliptical rod. The ratio of the major and minor axis is 1.25. Velocity is set to zero for all particles. After the simulation starts, the ellipse tends to transform into a circle to minimize its surface. However, due to the inertia of the liquid, the rod begins to oscillate, transforming surface and kinetic energy back and forth. The relation between the angular frequency of the oscillations Ω, surface tension coefficient σ, fluid density ρ, and the rod diameter D stands [9]

$$\Omega = \sqrt{\frac{48\sigma}{D^3\rho}} \tag{16}$$

The surface tension coefficient can be therefore calculated from the other parameters during the simulation, and the accuracy of a surface tension model can be evaluated by comparing the computed value with the nominal one.

In this work, the oscillation frequency is evaluated from measuring axes of the ellipse at discrete time instances and interpolating the data with the equation of dampened oscillatory motion using the least-squares method. Density is considered to keep its initial nominal value because it changes by less than 0.5%. A known volume of the rod serves for calculation of its diameter.

After the rod reaches its circular equilibrium state, the pressure profile is measured from the rod center to the surface and beyond. Virtual pressure sensors previously presented in [10] were used. The exact solution of pressure rise in a liquid rod due to surface tension is well known, so the model's precision can be evaluated again.

5. Results and Discussion

Three cases are presented, and the only changing parameter is the size (diameter) of the rod; all other physical and numerical parameters are kept constant. This parameter is considered to affect the model the most since the evaluation of surface normal vectors and curvature can be dependent on relative spatial resolution. The number of particles N in the discussed cases is 649, 1165, and 2259. Evaluation of the model is done by comparison between surface tension coefficient obtained using techniques described in the previous section and the nominal surface tension coefficient used in the model.

The measured oscillations and interpolation functions illustrates Fig. 1. Particles move orderly, which allows precise interpolation and thus reliable value of Ω. Oscillations are gradually dampened, but it does not affect the evaluation negatively. The ratio between evaluated and nominal surface tension coefficient varies from 1.023 for the smallest diameter to 0.958 for the largest one. One explanation for this is the fact that surface curvature is not evaluated exactly on the surface, but in a layer of finite thickness. The mean radius of this layer is lower than the surface radius, so the curvature is higher, and the effect of surface tension, according to the Young-Laplace equation (1), is greater. Relative layer thickness is higher for smaller diameter, and this effect is stronger.

The pressure inside the static rod for all three cases and the exact solution shows Fig. 2. The pressure in the rod is higher than predicts the exact solution by 12.4% for the lowest resolution and by 2.5% for the highest resolution. Resolution dependency can be again explained by surface layer thickness. Model behavior near the surface can be studied as well. Pressure drops in the surface layer from a constant value inside a rod to about 35% of this value on the very surface. The thickness of this layer depends on spatial resolution, and its thickness is about five times the initial particle spacing.

Overall, the static rod pressure test indicates higher values of surface tension coefficient than the oscillation test. The source of discrepancies between the two evaluation methods is probably due to different sensitivity to input parameters. For example, the surface tension coefficient directly proportional to D in the pressure evaluation, while in the oscillation method, it is proportional to D^3. Therefore, the oscillation method is more sensitive to any error in the determination of diameter. Table 1 summarizes the above-discussed results.

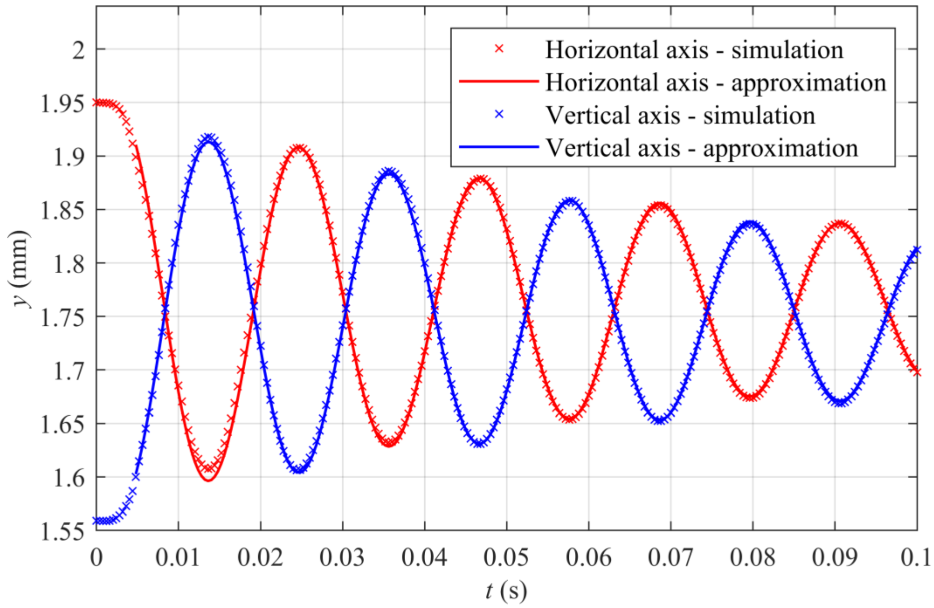

Fig. 1: Dimensions of axes of an elliptical rod as a function of time.

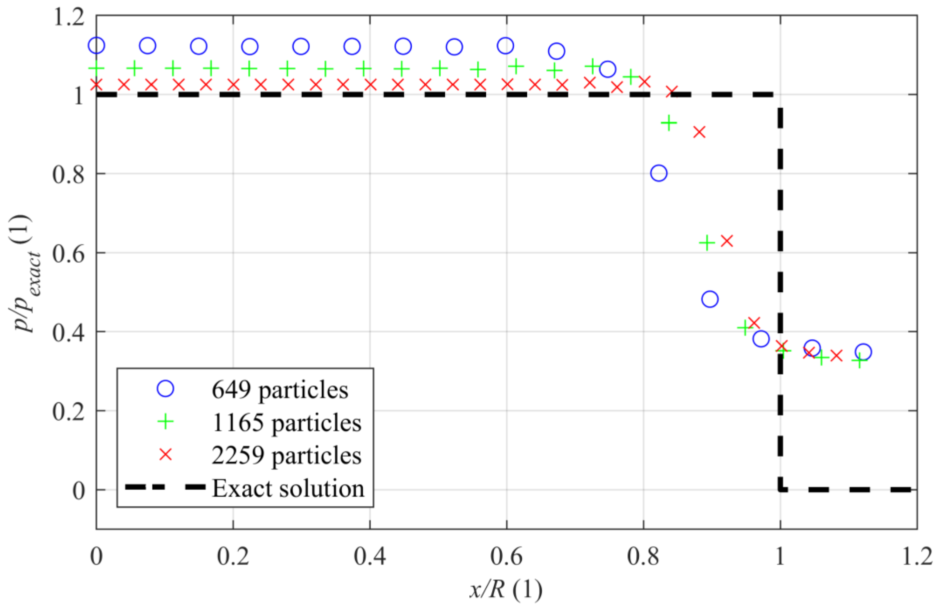

Fig. 2: Non-dimensional pressure as a function of non-dimensional distance from center of the rod; comparison of simulations and the exact solution.

Table 1: Summary of the discussed results.

N (1)	D (mm)	$\sigma_{oscillation}/\sigma_{model}$ [1]	$\sigma_{static}/\sigma_{model}$ [1]
649	1.338	1.023	1.124
1165	1.792	0.977	1.066
2259	2.495	0.958	1.025

6. Conclusion

The main goal of this paper is to propose a new CSF surface tension model for SPH suitable for free-surface and demonstrate its basic features on a simple two-dimensional problem. Two independent methods of evaluation were chosen for the validation of the model. Static rod internal pressure measurement is very straightforward and simple to while oscillation measurement, being a little more complex, gives information about surfaces in motion. The model itself to be stable and adequately precise for application to actual computational problems, for example, droplet interactions.

The model can be further improved, for example, by altering the color function transformation equation (8) and finding a more suitable one. The identified resolution dependency could be probably suppressed by correction on curvature evaluation based on distance from the surface.

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