Wetting phenomena and droplet-wall interaction modelling with Smoothed Particle Hydrodynamics approach

M Olejnïk and J Pozorski
Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Fiszera 14, 80-231, Gdański
E-mail: {michal.olejnïk, jp}@imp.gda.pl

Abstract. Smoothed Particle Hydrodynamics (SPH) is a meshless CFD method, remaining a promising alternative for multiphase flow calculations due to straightforward interface treatment. In the present work we particularly focus on the accurate modelling of wetting phenomena and contact angles. For that purpose we modify the surface tension model in the neighbourhood of the triple line. The necessity of proper boundary conditions in SPH is discussed along the preliminary validation of proposed approach. Results show a great potential of the chosen method.

1. Introduction
Wetting phenomena and interaction of droplets with different surfaces are fundamental processes governed by inertial, capillary and viscous forces. Accurate theoretical description and numerical modelling of such problems remain a difficult task, despite a superficial simplicity of the phenomena. The present work presents an attempt in tackling this challenge by means of the meshless Smoothed Particle Hydrodynamics (SPH) approach. SPH is the particle based method for fluid-flow modelling. Its Lagrangian nature and lack of numerical grid make it exceptionally suitable for cases where large deformations and topology changes occur, like interfacial flows. There is no need to track the interface or reconstruct it like in Eulerian approaches, since its position and shape can be explicitly obtained form positions of particles representing different phases. Furthermore SPH can handle large density ratios of liquid-gas systems fairly well. Examples of application of SPH to the problem of air bubbles rising in the liquid [1] or break-up of the liquid ligaments [2] show its usefulness as a multiphase flow solver. The present work is focused on the proper boundary conditions and contact angle treatment. To enable modelling of interactions of droplet with various type of surfaces we modify the interface normals used for surface tension forces calculations. The proposed method is tested for a range of static cases, with the preliminary study of a droplet in an air flow as a cherry on top.

2. SPH method for multiphase flows
SPH has been used for fluid dynamics problems for over twenty years, and many articles can introduce the Reader into the method, e.g. the review paper by Price [3] or comprehensive handbook by Violeau [4]. The general idea behind SPH lies in interpolation theory. If we
consider any field \( A \) defined on the space \( \Omega \), its value at point \( r \) can be interpolated from the integral
\[
A(r) \approx \int_{\Omega} A(r') W(r - r', h) d\Omega,
\]
where \( W(r, h) \) is the weighting interpolation kernel and \( h \) is the so called smoothing length, defining the range of interpolation (i.e. \( W(r, h) \equiv 0 \) for \( r \geq h \)). The discretisation of \( \Omega \) into a set of particles of volumes \( \Omega_b \) changes the integral in Eq. (1) into a summation, yielding basic SPH interpolation given as
\[
\langle A \rangle_a = \sum_b A_b W_{ab} \Omega_b,
\]
where \( W_{ab} = W(r_a - r_b, h) \), \( A_b = A(r_b) \) and \( a, b \) are indices of the SPH particles. Thanks to the properties of the kernel function the derivatives can be obtained by shifting differential operators from the fields to the function \( W(r, h) \). Approximation of gradient is simply taken as
\[
\langle \nabla A \rangle_a = \sum_b A_b \nabla W_{ab} \Omega_b,
\]
with higher derivatives obtained in analogous manner. Using this methodology differential equations can be translated into the SPH summation formulae and solved by calculating interactions between particles.

2.1. Governing equations
The set of the governing equations for viscous flow consists of the Navier-Stokes (momentum) equation
\[
\frac{d\mathbf{u}}{dt} = -\frac{1}{\varrho} \nabla p + \frac{\mu}{\varrho} \Delta \mathbf{u} + \mathbf{a}
\]
and the continuity equation
\[
\frac{d\varrho}{dt} = -\varrho \nabla \cdot \mathbf{u},
\]
where \( \mathbf{u} \) denotes the velocity vector, \( \varrho \) is the fluid density, \( p \) is the pressure and \( \mu \) is the dynamic viscosity. In Eq. (4), \( \mathbf{a} \) stands for the interfacial term, detailed in Sec. 2.2. Due to the Lagrangian nature of SPH we also include the advection equation for positions and velocities.

Depending on the purpose and assumptions, different SPH formalisms for the fluid flow can be obtained by using Eqs. (2) and (3). In the present study we use a formulation proposed by Hu and Adams [5]. To the best of our experience, their approach is best suited for modelling multiphase flows with large density ratios [6]. Due to limited space we will not present the SPH forms of governing equations, as they can be found in recent (and also decent) paper by Olejnik and Szewc [2]. The key feature of used formulation is replacing Eq. (5) with direct density calculation, i.e.
\[
\varrho_a = m_a \sum_b W_{ab}.
\]
This allows the density field to be represented only by the spatial distribution of particles and not by their masses. Thanks to this, densities of particles near the interface are not affected by the other fluid, which is important in multiphase flow modelling. In our work we use weakly compressible form of SPH, called WCSPH, hence the set of equations is closed with the equation of state
\[
p = \frac{s^2 \varrho_0}{\gamma} \left[ \left( \frac{\varrho}{\varrho_0} \right)^\gamma - 1 \right],
\]
where \( s \) is the artificial speed of sound, \( \varrho_0 \) is the reference (initial) density and \( \gamma \) is a numerical parameter. Values of \( s \) and \( \gamma \) are chosen to ensure density fluctuations at level of 1% or below.
2.2. Surface tension model

The influence of surface tension is modelled with Continuum Surface Force method (CSF), originally proposed by [7], with SPH implementation due to [8]. In this approach surface tension forces are converted into a force per unit volume

\[ F_s = f_s \delta_s = (\sigma \kappa \hat{n}) \delta_s, \]  

(8)

where \( \delta_s \) is a suitably chosen surface delta function, \( f_s \) is the force per unit area, \( \sigma \) is the surface tension coefficient, \( \kappa \) is the local curvature of the interface and \( \hat{n} \) is the unit vector normal to the interface. Using the so-called color function \( c \) (say, \( c = 0 \) for the first phase and \( c = 1 \) for the second one) \( \hat{n} \) can be calculated using the formula

\[ \hat{n} = \frac{n}{|n|} = \frac{\nabla c}{|\nabla c|}. \]  

(9)

The local curvature is obtained from

\[ \kappa = -\nabla \cdot \hat{n}. \]  

(10)

Assuming that \( \delta_s = |n| \), the influence of surface tension can be included in Eq. (4) by adding the term

\[ a_a = \frac{\sigma}{\rho_a} \kappa_a n_a. \]  

(11)

3. Boundary conditions and contact angle modelling

To accurately model wetting phenomena properly defined boundary conditions are of the essence. Lagrangian nature of SPH and use of moving particles as computational nodes makes modelling of solid wall a bit more challenging than in classic Eulerian approaches. The problem was intensively investigated for single phase flows, resulting in many schemes for boundary conditions to choose from. The most basic method is the so called dummy-particles approach, in which solid wall is built from immovable particles. The governing equations are solved for those “dummies”, but their positions and velocities are not evolved in time. This method works well despite its simplicity. However, for multiphase systems a simple question immediately arises – from which phase should the wall be built? The answer is by no means trivial. In the work of Yeganehdoust et al. [9] this approach was used for modelling the droplet-wall interaction. The colour function value for the dummies was derived from the temporary position of droplet, to allow for accurate calculation of the interface normals in the vicinity of the triple line. The proposed approach allowed for satisfactory results, but explicit tracking of the relative position of the droplet and the wall is problematic from the algorithmic point of view and limits versatility of the method.

In our work we use the so-called ghost particle approach for solid boundaries. In this method the wall acts as a mirror – each time step the particles close to the wall (at distance less or equal to the interpolation range of the kernel function used) are mirrored onto its opposite side. Their physical properties can be adjusted so that the desired boundary conditions, i.e. no-slip or free-slip, the Neumann b.c. for pressure, are satisfied. Detailed description of this approach can be found in [6] and [10]. In the case of multiphase flows the material properties of mirrored particles – density, viscosity and colour function, are exactly the same as those of parent ones. This is in fact very convenient, since (i) the boundary conditions are being constructed on the fly and there is no need for tracking the phase distribution in the flow; (ii) all summation formulae are calculated accurately without risk of under/overestimation of density or similar error. The main drawback of the ghost particles approach is its applicability only to cuboid domains, however, for the purpose of the basic research this is more than enough.

As for the contact angle calculation we decided to follow the idea used in the Volume of Fluid approach by Sikalo et al. [11]. We modify the unit vector normals to the interface near the
triple line as
\[
\left[ \frac{\nabla c}{|\nabla c|} \right]_{\text{mod}} = n_\perp \cos \theta_D + n_\parallel \sin \theta_D,
\]  
where $\theta_D$ is the desired contact angle whereas $n_\perp$ and $n_\parallel$ are the unit vectors perpendicular and parallel to the wall, see Fig. 1. By “near the triple line” we mean particles that satisfy the following conditions: (i) they are closer than $2h$ from the wall; (ii) they have a non-zero $\nabla c$. The choice of $2h$ is simply the range of the kernel function employed in our calculations. Equation (12) is used for curvature calculation only, hence Eq. (11) becomes for these particles
\[
a_a = \frac{\sigma}{\varrho_a} \left( -\nabla \cdot \left[ \frac{\nabla c}{|\nabla c|} \right]_{\text{mod}} \right) n_a.
\]  
To avoid problems with a non-smooth transition from the modified to primal vectors normal to the interface, we employ the correction proposed by Breinlinger et al. [12]
\[
\left[ \frac{\nabla c}{|\nabla c|} \right]_{\text{mod}} = \alpha (n_\perp \cos \theta_D + n_\parallel \sin \theta_D) + (1 - \alpha) \frac{n}{|n|},
\]  
where $\alpha$ is the linear blending function equal 0 on the wall and 1 at the distance $2h$ apart. The described model is very robust, and, as proved in Sec. 4., can yield accurate results.

We also need to stress that within the ghost particles approach framework, the solid wall is not physically present in the calculations. Due to the formulation, the particles are not penetrating it or getting exactly to its position. This means that there are no issues related to the no-slip boundary condition and velocity following from the acceleration computed in Eq. (13).

4. Results
4.1. Static cases
The model was first applied to the 2D static case. The initially hemispherical droplet of liquid was placed on the wall as in the first panel of Fig. 2. The density and viscosity ratios of gas $G$ and liquid $L$ were set to $\varrho_L/\varrho_G = 1000$ and $\mu_L/\mu_G = 100$, respectively. The resolution was set to $h/R = 1/16$ and $h/\Delta r = 2$, where $R$ is the initial radius of the droplet and $\Delta r$ is the mean spacing between particles. Only surface tension forces were inducing the motion (no gravity or another forcing). The domain was periodic in the left-right direction and high enough to ignore the influence of the top wall and with no-slip b.c. on the bottom. The model was tested for values of $\theta_D$ ranging from $30^\circ$ to $150^\circ$. Due to the modification of the interface normals near the triple line and resulting acceleration, the droplet should spread on the wall or minimise its contact area, depending on the value of $\theta_D$. As shown in Figs. 2 and Fig. 3 this is exactly what happens. In both cases the droplet will finally reach the desired shape and the modified vectors

![Figure 1. Schematic illustration explaining the way in which interface normals are modified.](image)
Figure 2. Evolution of the droplet placed on a hydrophilic wall ($\theta_D = 30^\circ$).

Figure 3. Evolution of the droplet placed on a hydrophobic wall ($\theta_D = 150^\circ$).

Figure 4. Comparison of the steady-state solution for different values of $\theta_D$. The black line marks isoline of the colour function 0.5.

will be equivalent to those of the CSF model, and the motion will cease. Figure 4 shows a result obtained for the whole range of the $\theta_D$ tested. What is curious, but also expected, applying no special treatment yields the same result as imposing $\theta_D = 90^\circ$.

4.2. Dynamic cases
As was already mentioned, the model does not pose any problems related to the contradiction between no-slip b.c. and triple line velocity, hence we applied it to the dynamic case. We modelled exactly the same set-up as in previous Sec. 4.1, but with increased resolution ($h/R = 1/32$ and $h/\Delta r = 2$). Furthermore, the mass force was imposed along the channel’s length to induce the motion. The computations were performed for two values of $\theta_D$, namely $30^\circ$ and $150^\circ$, to model the interaction of droplet with entirely different walls. In both cases the creeping air flow forced movement of the droplet. The dimensionless numbers defined with the mean velocity at the channel centreline were $Re < 1$ and $Ca \approx 1$. As expected, for the hydrophilic wall we observed smearing of the droplet, as shown in the upper panel of Fig 5. In
Figure 5. Evolution of the liquid droplet (royal blue and green) in the creeping gas flow (light blue and revolutionary red). Upper panel - hydrophilic wall, bottom - hydrophobic. The gas flow direction is from left to right.

the case of the hydrophobic wall, droplet started to steadily roll, which is also in agreement with physical intuition.

5. Conclusions
In the present study we have presented a robust, yet effective method of the wetting phenomena modelling within the framework of ghost particles boundary conditions for SPH. The model was able to capture wide range ($30^\circ - 150^\circ$) of the desired static contact angle. Simulation of the droplet placed on the wall, subjected to the air flow, yielded satisfactory results. The outlook for future development is promisingly bright. The next step of the research should focus on moving into the 3D set-up (which will be straightforward) and thorough, quantitative validation. Based on the problems and inaccuracies encountered we will further improve the model.

Acknowledgements
This research was partly supported by the National Science Center (2013/11/B/ST8/03818).

References
[1] Szewc K, Pozorski J, Minier J-P 2013 Int. J. Multiphase Flow 50 98
[2] Olejnik M, Szewc K 2018 J. Theor. App. Mech. (Pol.) 56 in press
[3] Price DJ 2012 J. Comp. Phys. 231 759
[4] Violeau D 2012 Fluid Mechanics and the SPH Method (Oxford: Oxford University Press)
[5] Hu XY, Adams NA 2006 J. Comp. Phys. 213 844
[6] Szewc K, Pozorski J, Minier J-P 2012 Int. J. Num. Meth. Eng. 91 343
[7] Brackbill JU, Kothe DB, Zemach C 1992 J. Comp. Phys. 100 335
[8] Morris J P 2000 Int. J. Num. Meth. Fluids 33 333
[9] Yeganehdoust F, Yaghoubi M, Emdad H, Ordoubadi M 2016 App. Math. Model. 40 8493
[10] Cummmins SJ, Rudman M 1999 J. Comp. Phys. 152 584
[11] Šikalo Š, Wilhelm HD, Roisman IV, Jakirlić S, Tropea C 2005 Phys. Fluids 17 062103
[12] Breinlinger T, Polfer P, Hashibon A, Kraft T 2013 J. Comput. Phys. 243 14