A multi-physics single-phase SPH scheme to simulate droplet migration on a heated solid surface

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I. INTRODUCTION

This work presents a single-phase smoothed particle hydrodynamics (SPH) scheme capable of simulating droplet migration on a heated solid surface. The scheme is implemented in the DualSPHysics [1] open-source weakly compressible SPH (WCSPH) multi-physics (CFD) solver.

When a droplet is placed on a heated surface with a temperature gradient, the droplet will become mobile driven by the Marangoni effect. This phenomenon has attracted many researchers because it can be applied to various droplet-based fluidic devices in industry [2].

Due to the diverse length and timescales, arising from the small length scale and high mobility of the droplet, the SPH method is highly appropriate thanks to its Lagrangian mesh-free formulation and suitability for free-surface flows compared to the traditional mesh-based CFD methods.

Droplet migration is rarely studied using SPH. Recently, Long *et al.* [3] developed an improved SPH method to study the droplet migration under varying contact angles and viscosities, showing good agreement with the experimental data. However, their results showed a deviation between the numerical and experimental results and lacked 3-D simulations. To address these limitations, this work provides a more accurate estimation of displacement and 3-D results for droplet migration.

II. NUMERICAL METHOD

The single-phase weakly-compressible SPH scheme used in this work includes a single-phase surface tension model [4-5], Marangoni effects [6], Oberbeck-Boussinesq (OB) buoyancy approximation, heat transfer [7], an acoustic damper term [8] all incorporating into the open-source SPH solver DualSPHysics [1].

This work starts from the formulation of Cen et al. [5] with the addition of multiple new physics including: the heat transfer scheme from Cleary and Monaghan [7], Marangoni forces from Bierwisch [6], the OB buoyancy approximation, and the acoustic damper term from Sun *et al.* [8]. To improve the particle distribution, the optimized particle shifting methods (OPS) from Khayyer et al. [9] is also applied in this work. Finally, the recently extended no-slip version of mDBC is used [10]. To the best of the authors' knowledge, this is the first time these models have been combined together for a multi-physics application.

III. RESULTS AND DISCUSSION

To validate the scheme, different benchmarks for the sub-models in the proposed scheme are conducted including the droplet impact on a solid surface and natural convection in a heated cavity. Finally, the droplet migration on a heated solid surface is demonstrated.

A. Droplet impact on a solid surface

Two test cases examining the dynamic evolution of a single droplet impacting on a solid surface are presented here with low to moderate Reynolds numbers. The experimental parameters are shown in Table 1 reproduced from the reference paper of Šikalo *et al.* [11].

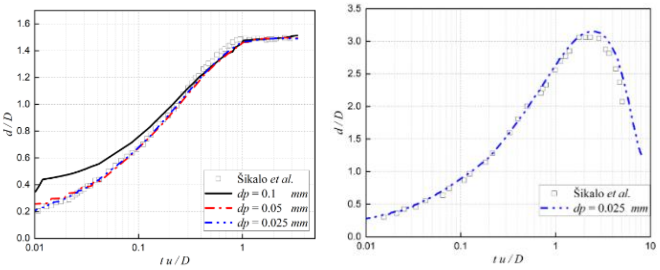
Table 1: Parameters of the cases adopted from Šikalo et al. [11].

Parameters	**Test 1**	**Test 2**
Fluid	Glycerin	Water
Density	1220 kg/m^3	996 kg/m^3
Dynamics viscosity	0.116 Pa·s	0.001 Pa·s
Surface tension	0.063 N/m	0.073 N/m
Equilibrium angle	95°	100°
Impact velocity	1.04 m/s	1.64m/s
Weber number	51	90
Reynolds number	27	4010

First, a low Reynolds number case with *Re* = 27, where a glycerin droplet impacts on a solid wax surface, is presented. Three initial inter-particle distances are chosen as *dp* = 0.1, 0.5 and 0.025 mm, giving 9563, 48420 and 514255 fluid particles, respectively. The spreading factor *d/D*, which is the ratio of the spreading diameter d to the initial diameter of the droplet D, is compared between the SPH result and the experimental data from the reference as shown in Figure 1-(a). It is found that the SPH result converges to the reference result. This test case proves that the current model is able to accurately describe the droplet impact case with the relatively low Reynolds number.

The case with Re = 4010 is presented next. It is found that additional techniques to the classical SPH should be applied in this case to ensure the stability and accuracy of the test case. At first, the acoustic damper term [8] is used to reduce the acoustic pressure. This helps suppress the ejection of particles at the edge of the lamella when the droplet contacts the surface. Secondly, in addition to the laminar viscosity term, the artificial viscosity is also required to stabilise the fluid, where the typical coefficient α = 0.02 is adopted based on our experience. The requirement of an additional viscous term is to be expected, as the Riemann solver scheme used in [4] provides additional numerical diffusion. It is noted that the artificial viscous coefficient should be calibrated for a specific case as the diffusion in Riemann solver is implicitly adopted therefore a quantitative analysis cannot be performed and compared. Similar to the effect of the acoustic damper term, the artificial viscosity helps to avoid the ejection of particles during impact. Besides, it can also help with the prevention of the separation of the lamella from the droplet disk. Thirdly, the shifting criterion from Sun et al. [12] is adopted, where the particle shifting technique is switched off for free-surface particles with the minimum eigenvalue less than 0.4. This is because the particle shifting technique can induce spurious numerical effects for such free-surface particles whose normal vectors might be inaccurately estimated due to the incomplete kernel support [12]. Finally, a more restrictive criterion is added for the normal identification, where the normal for the interior particles is set to 0. This is because we find that there is a very thin air film between the lamella and the solid surface during the droplet impact and spreading process, which is physical [13], numerically leading to the overestimation of the gradient of the minimum eigenvalue in the case of the single-phase model. As a consequence, the normal of a few interior particles located at the bottom of the lamella may not be strictly 0, resulting in the existence of the surface tension on these particles and introducing errors.

In this case, we first attempted the same initial inter-particle distances of dp = 0.1, 0.05 and 0.025 mm. However, unexpected break-up behaviour is observed even though the above methods are applied for the cases with dp = 0.1 and 0.05 mm. This breakup might be owing to the very thin film where the small number of particles within such film are not able to capture the film behaviour. The breakup does not occur in the case with dp = 0.025 mm because there are sufficient particles in the film. Similarly, the spreading factor profile is shown in Fig. 1-(b) and a good agreement is obtained where the relative error of the maximum spreading factor is around 3%.



(a) (b)

Figure 1. Profile of spreading factor d/D for (a) glycerine droplet case (b) water droplet case.

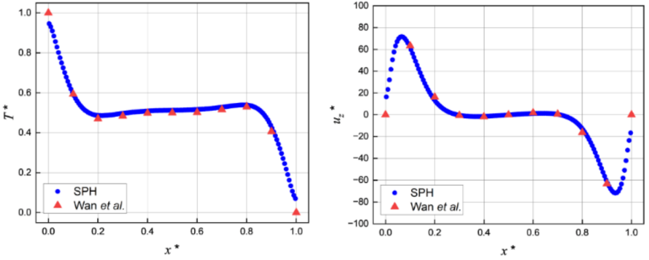
B. *Natural convection*

A natural convection test case is used to validate the heat transfer model and OB approximation. Based on the relevant setup of natural convection case in Reece [14], air within a cavity with room temperature T_{air} = 293 K, Pr = 0.71 and Ra = 10^5 is chosen to be compared with the result in Wan *et al.* [15]. The left wall at x = 0 m (T_{hot} = 303 K) and right wall at x = 0.04 m (T_{cold} = 283 K) hold a constant temperature during the simulation using a Dirichlet boundary condition so that the temperature difference is fixed at 20K. The top and bottom walls are adiabatic so that the physical boundary condition to be imposed is $\partial T/\partial z = 0$ as a Neumann boundary condition. The length of the cavity is L = 0.04 m and the particle spacing is chosen as dp = 0.25 mm which gives 25600 fluid particles. The relevant parameters are shown in Table 2. The fluid particles have an initial uniform temperature distribution of T_{air} = 293 K which is also the reference temperature in the OB term.

Table 2: Parameters of the natural convection case

Parameters	**Value**
Density	1.204 kg/m^3
Kinematic viscosity	1.506·10^{-5} m^2/s
Heat capacity	1006 J/(kg·K)
Heat transfer coefficient	0.02587 W/(m·K)
Thermal expansion	0.00343 K^{-1}
Gravity	(0, 0, -8.821 m/s^2)

The results are compared to Wan *et al.* [15] where a high-order discrete singular convolution method is introduced to investigate buoyancy-driven problems. The dimensionless temperature and the vertical velocity along the horizontal mid-line are shown in the Figure 2. The SPH results are obtained by the interpolation measure tool in DualSPHysics. It can be seen that the SPH results agree well with that of Wan *et al*. [15]



(a) (b)

Figure 2. Results of natural convection (a) dimensionless temperature along mid-line (b) dimensionless velocity along mid-line.

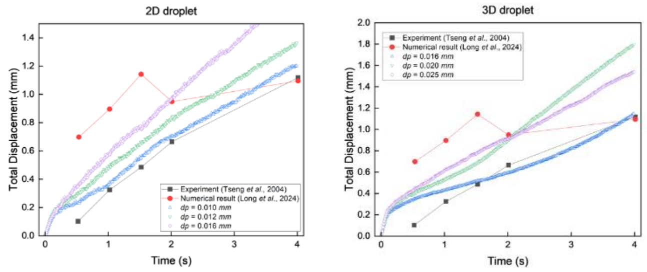
C. *Droplet migration*

The droplet migration case driven by temperature gradients in both 2-D and 3-D are investigated here. Following the numerical study from Long *et al*. [3] and the experimental study from Tseng *et al*. [16], the fluid properties are presented in Table 3. As the Marangoni effect is partially suppressed in physical experiments due to unavoidable surfactants being present, the Marangoni coefficient was reduced to 20% of the physical value to reduce the numerical overestimation. The temperature profile of the surface is extracted from the reference [16].

Table 3: Parameters of the droplet migration

Parameters	Value
Density	963 kg/m^3
Dynamic viscosity	0.04 Pa·s
Heat capacity	1670 J/(kg·K)
Heat transfer coefficient	1 W/(m·K)
Thermal expansion	0.00343 K^{-1}
Surface tension	0.024 N/m
Marangoni coefficient	0.0094 mN/(m·K)
Equilibrium contact angle	53°
Inter-particle distance in 2-D	0.01, 0.012, 0.016 mm
Inter-particle distance in 3-D	0.016, 0.02, 0.025 mm

Figure 3 shows the displacement increment compared with the experimental results [16] and the numerical results [3] in 2-D and 3-D. It can be observed that the 2-D results converge to the experimental results, while the 3-D results do not exhibit strict convergence behaviour. One possible reason is that when the droplet initially starts to move, the sudden Marangoni force induces a large velocity, which can be observed in both the 2-D and 3-D cases. Another reason could be the use of a no-slip boundary condition in the simulation, whereas a slip boundary condition would be more appropriate to match reality. This remains to be further investigated.



(a) (b)

Figure 3. Total displacement of droplet migration case in (a) 2-D and (b) 3-D.

IV. CONCLUSION

In this work, a single-phase SPH scheme capable of modelling the droplet migration on a heated solid surface has been developed.

The droplet impact on a solid surface and the natural convection are applied to validate the scheme. The numerical results agree well with the reference where the relative error is around 3-5%. Then, the behaviour of the droplet migration in both 2-D and 3-D is investigated. Under the effect of the temperature gradient, the droplet moves towards the cold region. The total displacement converges and agrees well with the experimental results. However, the sudden Marangoni force and the unmatched boundary condition introduce error to both 2-D and 3-D cases. Further research will focus on these two aspects.

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