Modeling Footprint Profiles for Different Drop-Substrate Pairs

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Abstract—Modeling drop dynamics in 3D is an active area of research. Of particular interest is the simulation of the contact line profiles for moving liquid drops of varying physical properties, such as liquid surface tension and substrate wettability. The Lagrangian Particle Finite Element Method (PFEM) numerical approach is adopted for predicting the footprint profiles of moving liquid drops. The Lagrangian PFEM is advantageous due to its ability to provide an accurate mesh-based boundary description, and thus, facilitates the computation of the free-surface and footprint evolution. The modeling outcomes agree with the general experimental behavior for different drop-substrate pairs with widely differing properties.

Index Terms—Droplet footprint, Lagrangian PFEM, Wetting phenomena, Surface tension, Contact line profile

I. INTRODUCTION

The effect of surface wettability on the spatio-temporal evolution of a liquid drop is important in every aspect of life. For instance, the spatio-temporal evolution mechanism of water drops in biological and agricultural systems is one of the most important resources for plants and beetle to survive [1]. The hydrophobicity of the lotus leaves causes water droplets to repel from their surfaces, and turns out to be a drinking water source for other organisms. This also facilitates contaminant particle removal, and, in turn, endows the leaf with its self-cleaning ability [2, 3]. In contrast, the hydrophilicity of stipagrostis sabulicola leaves guides water droplets down towards its roots [4, 5, 6]. In the field of bioengineering, predicting the sliding mechanism of blood drops, i.e., hemophobicity analysis, promotes the control of coagulation and contamination in blood-contacting medical devices [7, 8]. With the evolution of micro- and nanofabrication techniques, scientists have utilized the natural wetting phenomena to develop the manufacturing of surfaces with custom-made wetting properties [9]. For instance, liquid drops on higher hydrophobicity substrates have been proven to be functional and efficient for self-cleaning applications and devices [10, 11].

This paper extends the previous work of [12, 13, 14], and aims at modeling the footprint profile for sliding liquid drops. The moving grid Lagrangian Particle Finite Element Method (PFEM) [15] has been adopted in the proposed model, as it has proven to be an effective and accurate approach for modeling drop dynamics problems with evolving domains [14, 16, 17].

This paper is structured as follows: The following section introduces the physical model and mathematical formulation for a moving liquid drop on a solid substrate, followed by the numerical implementation and three-dimensional mesh dependency analyses in Section III. The numerical findings are discussed in Section IV, followed by the conclusion in Section V.

II. MATHEMATICAL MODEL

A. Governing equations

Let \( \Omega \) represent the domain of the liquid drop. Let \( \Gamma_I \) be the free-surface of the liquid drop, \( \Gamma_S \) be the liquid drop in contact with the solid substrate excluding the contact line, and \( \partial \Gamma \) be the contact line. Consequently, the domain boundary, i.e., \( \partial \Omega \), is divided into \( \Gamma_I \cup \partial \Gamma \cup \Gamma_S \), as illustrated in Fig. 1.

The liquid drop is assumed to be an incompressible Newtonian fluid. Accordingly, the governing momentum and mass conservation equations are expressed as follows: [16, 18]:

\[
\rho \frac{Dv}{Dt} - \mu \nabla \cdot (\nabla v + \nabla^T(v)) + \nabla p = \rho g \quad \text{on} \quad \Omega \\
\nabla \cdot v = 0 \quad \text{on} \quad \Omega
\]

where \( \rho \) is the density, \( v \) is the velocity field, \( t \) is time, \( \mu \) is the dynamic viscosity, \( p \) is the pressure, and \( g \) is the gravitational acceleration.
B. Boundary conditions

At $\Gamma_f$, where the surface tension force ($f_{\Gamma_f}$) exists, the Cauchy stress condition is applied in the normal direction as follows:

$$f_{\Gamma_f} = \sigma n = \gamma k_h n \quad \text{at} \quad \Gamma_f$$

(3)

where $\sigma$ and $k_h$ stand for the Cauchy stress tensor and the mean curvature of the free-surface, respectively. $\gamma$ stands for the surface tension coefficient and $n$ is the outer unit normal to the free-surface. More details about Cauchy stress tensor $\sigma$ for drop dynamics modeling can be found on reference [14].

At $\partial\Gamma$, the slip velocity of the contact line is proportional to Young’s stress acting on it:

$$v \propto (\cos \theta_r - \cos \theta_s) \quad \text{at} \quad \partial\Gamma$$

(4)

where $\cos \theta_r$ and $\cos \theta_s$ stand for the static and dynamic contact angles. An effective slip condition ($\beta_{\partial\Gamma}$) is imposed to account for Young’s stress and the associated dissipative forces ($f_{\partial\Gamma}$) acting on the contact line, which includes: i) the capillary force coefficient ($\beta_c$), ii) the normal stress coefficient ($\beta_n$), and iii) the Navier-slip coefficient ($\beta_s$). Thus, the coefficient $\beta_{\partial\Gamma}$ is proportional to the velocity of the contact line as follows [19, 20, 21, 22, 23]:

$$f_{\partial\Gamma} = -\beta_{\partial\Gamma} v = - (\zeta + \beta_c [\partial\Gamma] + \beta_n) v \quad \text{at} \quad \partial\Gamma$$

(5)

As the liquid drop slides, the impact of a retention force on the contact line is also taken into account. The quantity of this retention force can be predicted as follows [24, 25, 26]:

$$F_{\text{Retention}} = \gamma k a (\cos \theta_R - \cos \theta_A)$$

(6)

where $k$ is a function of the drop footprint’s aspect ratio and $a$ is the wetting radius. The values $\theta_R$ and $\theta_A$ correspond to the receding and advancing contact angles, respectively. The retention force works against the gravitational force when a liquid drop slides under its own weight. More details about the retention force can be found in reference [14].

As the liquid drop deforms, Navier-slip condition is applied at $\Gamma_S$ to account for the viscous dissipation at the solid-liquid interface away from the contact line [21, 22]:

$$f_{\Gamma_S} = -\beta_{\Gamma_S} v \quad \text{at} \quad \Gamma_S$$

(7)

where $f_{\Gamma_S}$ and $\beta_{\Gamma_S}$ are the viscous dissipative force and the applied slip coefficient on $\Gamma_S$, respectively [14].

III. NUMERICAL IMPLEMENTATION

The Updated Lagrangian Fluid formulation within Kratos Multi-Physics software is used for the numerical implementation [27]. The Second-order Backward Difference scheme is used for the time discretization [28]. More details about the discretization can be found in reference [12, 14].

On one hand, the Lagrangian PFEM approach is advantageous for accurately tracking the surfaces and the contact line. On the other hand, it is costly in 3D due to extensive remeshing requirements. One solution is utilizing the adaptive meshing concept, especially at the contact line.

Figure 2 shows the numerical simulation output for water drops evolving from different initial configurations, using different mesh sizes. The results indicate the importance of the adaptive mesh concept in obtaining final accurate configurations of the boundaries.

IV. RESULTS AND DISCUSSION

To examine the proposed Lagrangian PFEM model for predicting the footprint profile of a variety of moving liquid drops on different substrates, this section looks at three experimental scenarios that were taken from the published literature. Table I lists the liquid drop’s physical characteristics for various liquid-solid combinations.

- Case #1: the first validation examines the contact line profile for an ethylene glycol (EG) drop of 29.9$\mu$L volume, sliding on an omniphilic polycarbonate surface. The surface’s angle of inclination is considered as $\alpha = 20^\circ$ [25]. Experimental results reveal the value of $k$ to be 1.41 [29]. The physical characteristics for the first case of Table I are used to run the simulation. The values of the mesh size and time step are set to be $4 \times 10^{-4}$ m and $8 \times 10^{-5}$ s (see reference [14] for the mesh size and time steps criteria).

- Case #2: the second validation examines the contact line profile for a viscous Newtonian polyethylene glycol (PEG) drop of 100$\mu$L volume, sliding on a hydrophobic polytetrafluoroethylene (PTFE) substrate. A 60$^\circ$ inclination angle is used for the water drop’s slide. [30]. The numerical simulation is implemented using the physical characteristics for the second case of Table I. Experimental results indicate that the value of $k$ is 1.35 [29]. The mesh sizes and time steps are set to be $1.1 \times 10^{-4}$ m and $10^{-5}$ s.

- Case #3: the third validation examines the contact line profile for an ethylene glycol (EG) drop of 29.9$\mu$L volume, sliding on a smooth glass omniphilic substrate. The PEG drop slides at an inclination angle of 27$^\circ$ [31]. A value of 2.0 is selected for $k$ [31]. The numerical simulation is implemented using the physical characteristics for the last case of Table I. Due to the relatively large volume of the drop, an adaptive mesh size of $9 \times 10^{-4}$ m is refined at the boundaries to $6 \times 10^{-4}$ m. The time step is set to be $10^{-4}$ s.

The numerical steady-state values of the three cases were found to be in agreement with the experimental results with an average relative error of 8% (see reference [14] for more details). Detailed discussion about the footprint profiles for these liquid-solid pairs is discussed next.
TABLE I. PHYSICAL CHARACTERISTICS OF THREE DIFFERENT LIQUID-SOLID PAIRS.

<table>
<thead>
<tr>
<th>Case</th>
<th>Liquid drop</th>
<th>Substrate</th>
<th>ρ (kg m⁻³)</th>
<th>µ (Pa s)</th>
<th>γ (N m⁻¹)</th>
<th>θ (°)</th>
<th>k</th>
<th>t</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>EG</td>
<td>polycarbonate</td>
<td>1114</td>
<td>2.09 x 10⁻²</td>
<td>4.84 x 10⁻²</td>
<td>70.2</td>
<td>1.41</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>water</td>
<td>PTFE</td>
<td>997</td>
<td>8.9 x 10⁻⁴</td>
<td>7.28 x 10⁻²</td>
<td>120</td>
<td>1.35</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>PEG</td>
<td>glass</td>
<td>1080</td>
<td>2.5 x 10⁻¹</td>
<td>5.33 x 10⁻²</td>
<td>34.0</td>
<td>2.0</td>
<td></td>
</tr>
</tbody>
</table>

A. Footprint profiles for different liquid-solid pairs

According to the omniphilicity of the substrate and its tilted angle, three different footprint profiles can be observed as a liquid drop begins to slide [29, 32]. A sliding drop on an omniphobic substrate has a front-to-back symmetrical footprint profile. However, a parallel-side or a back-to-front symmetrical footprint profile can be observed for drops sliding on omniphilic substrates (see Fig. 3). Fig. 4 shows different reported experimental footprint profiles for different liquids drops sliding on a variety of substrates [29, 32, 33].

Due to the lack of full details of experimental conditions of Fig 4, the validity of the qualitative behavior of the footprint obtained numerically is examine using the three scenarios of Table I. The results are shown in Figs. 5-7. The qualitative behavior is in very good agreement with what has been observed experimentally for varieties of liquid drops sliding on different substrates (shown in Fig 4). In Fig. 5, parallel side symmetry was observed for the small EG drop moving on the omniphilic polycarbonate surface. Unlike the sliding liquid drop on an omniphilic solid substrate, the advancing contact line is narrower than the receding one for a sliding drop on inclined omniphobic substrates (Fig. 6). In addition, tails are expected to appear for large sliding drops on omniphilic substrates, as depicted in Fig. 7.

V. CONCLUSION

The proposed Lagrangian PFEM numerical simulations were able to predict the dynamics of moving liquid drops, including their footprint profiles. As the drop starts to slide, its footprint profile is shaped in accordance with i) the volume and viscosity of the drop, and ii) the omniphilicity of the substrate. For instance, front-to-back symmetry was observed for liquid drops sliding on omniphobic substrates. Parallel-side symmetry was observed for small viscous drops sliding on omniphilic substrates. Tails were observed for liquid drops sliding on omniphobic substrates. The proposed three-dimensional model can be extended to study the dynamics of a moving liquid drop and its footprint profile for an embedded two-phase flow, considering different liquid-solid pairs.
Fig. 4. Footprint profiles for: (a) 116µL water drop sliding on a hydrophobic PCTFE substrate (front-to-back symmetry) [29], (b) 3µL EG drop sliding on an omniphilic polyethylene surface (parallel-side symmetry) [34], (c) a millimeter-sized drop of viscous silicon oil sliding on an omniphilic smooth glass (back-to-front symmetry) [32], (d and e) 15µL viscous bromonaphthalene drop sliding on an omniphilic aluminum substrate at different inclination angles (parallel-side symmetry and back-to-front symmetry) [33].

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Fig. 5. A 29.2µL ethylene glycol (EG) drop sliding on an omniphilic polycarbonate substrate: (a) contact angle distribution, and (b) plane view of a parallel-slide footprint profile.

Fig. 6. A 7.5µL water drop sliding on a hydrophobic polytetrafluoroethylene (PTFE) substrate: (a) contact angle distribution, and (b) plane view of a front-to-back symmetrical footprint profile.
Fig. 7. A 100µL viscous Newtonian polyethylene glycol (PEG) drops sliding on an omniphilic smooth glass substrate: (a) contact angle distribution, and (b) plane view of a back-to-front symmetrical footprint profile.

REFERENCES


