DROPLET SPREADING BEHAVIOUR OVER A SOLID SUBSTRATE MEDIATED BY SURFACE WETTABILITY AND INTERFACIAL TENSION

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ABSTRACT

The present study investigates the fluid-solid interaction phenomenon when a spherical droplet falls on the surface of a solid substrate. Numerical investigations were carried out in a 2D framework to analyse the influence of the wettability of the substrate and interfacial tension of the liquid droplet. The 2-D solver establishes a good agreement with the reported experimental results. The droplet is considered to fall on the solid surface under the influence of a minimal velocity imposed on it. The results are presented in terms of droplet interface morphology and the spreading distance over the solid substrate. It is observed that the spreading tendency of a droplet is much more significant with a hydrophilic surface compared to a hydrophobic surface. It is also established that with the decrease in Weber number the droplet spreading increases. However, droplet spreading on a hydrophobic surface increase with the decrease in Weber number up to a certain limit, after which the droplet starts to contract, reducing the droplet spreading on the surface.

Keywords: Droplet spreading, hydrophilic, hydrophobic, solid substrate, Weber number, wettability.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
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<tbody>
<tr>
<td>D</td>
<td>[mm]</td>
<td>diameter of the droplet</td>
</tr>
<tr>
<td>Lₙ</td>
<td>[-]</td>
<td>non-dimensional spreading length</td>
</tr>
<tr>
<td>We</td>
<td>[-]</td>
<td>Weber number</td>
</tr>
<tr>
<td>θ</td>
<td>[degree]</td>
<td>contact angle</td>
</tr>
<tr>
<td>μ</td>
<td>[Pa s]</td>
<td>viscosity</td>
</tr>
<tr>
<td>ρ</td>
<td>[kg/m³]</td>
<td>density</td>
</tr>
<tr>
<td>σ</td>
<td>[N/m]</td>
<td>surface tension</td>
</tr>
<tr>
<td>τ</td>
<td>[-]</td>
<td>non-dimensional time</td>
</tr>
<tr>
<td>ϕ(x,t)</td>
<td>[-]</td>
<td>level-set function</td>
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1. INTRODUCTION

When a droplet impacts on a solid surface, the dynamics of interfacial characteristics becomes complex. Researchers have found the dynamics of a droplet impacting on a substrate a topic of interest owing to its appealing physics and versatile applications like ink-jet printing [1], pesticide depositions [2], impact erosion [3], anti-icing [4], etc.

Droplet impact on a solid substrate takes many forms (e.g., spreading, bouncing, fingering, splashing, etc.) [5] based on different properties of the surface as well as different physiochemical and flow properties of the fluid. These include the surface properties of roughness [6] and wettability [7], while fluid properties such as interfacial tension, viscosity, density, and impact velocity [8-10] are some of the key determinants of droplet impact over a solid surface.

The spreading of a liquid droplet on a specifically wetted surface has drawn attention from the research community for bearing remarkable potential within the domain of biomedical research, microfluidics, lab-on-chip applications, etc. The key parameters that govern the phenomenon of spreading over a solid substrate are dynamic contact angle, impact velocity of the droplet and topology of the solid-liquid contact line. Researchers have reported that the dynamic contact angle is dependent upon the physical structure of the impacting surface [11], interfacial characteristics of the participating liquid [12] and also the method by which the droplet is let to impact over the surface [13, 14]. Wildeman et al. [15] investigated numerically and analytically the spreading behaviour of droplet over a smooth surface when the droplet impacts the surface at a high velocity. They found that during the spreading of a liquid droplet over the free-slip surface one-half of the kinetic energy is converted to interfacial energy, irrespective of any other flow parameters. Lann et al.
[16] experimentally explored the influence of impacting droplet diameter on spreading over a solid surface. They reported that the spreading characteristics of the droplet not only depend on the inertia, viscous or capillary force, but also on the droplet size and provide an accurate scaling of droplet spreading behaviour. Léopoldès and Bucknall [17] identified three distinct regimes of droplet spreading when a solid surface is differentiated with two micro-stripes having definite wettability contrast. In their study, different spreading behaviours of droplet were analysed with the variation of wettability contrast. In another study carried out by Kuznetsov et al. [18], three different spreading regimes were identified for a distilled water droplet impacting a solid superhydrophobic and copper substrate.

The dynamics of a droplet when it is imposed with a certain velocity can be characterised by a non-dimensional similarity number called Weber number \((W)\), which represents the relative importance of velocity with respect to the surface tension of the liquid. Liu et al. [19] investigated the spreading characteristics of a droplet over a surface at low Weber numbers. Shang et al. [20] explored the spreading of a droplet for a range of Weber numbers on a solid surface maintained at a very low temperature. They reported that a low Weber number leads to a decrease in spreading length, with spreading length first decreasing and then increasing with subsequent cooling at higher Weber numbers.

Most of the recent studies on the spreading of a liquid droplet over a solid surface have explored the influence of surface wettability and a few key determinants like impact velocity, viscosity or surface tension. However, the combined effect of surface wettability with a low Weber number on the spreading characteristics is yet to be studied. Thus, the present study aims to investigate the spreading behaviour of a liquid droplet on a solid surface of different wettability conditions for a specific range of Weber numbers.

2. THEORETICAL FORMULATION

2.1. Problem formulation

The present study numerically investigates the spreading behaviour of a liquid droplet over solid substrate under the combined influence of the wettability condition of the substrate surface, the initial velocity of the droplet and the interfacial tension. A two-dimensional computational domain is used (see Fig. 1) in the present investigation in order to reduce the cost of computation, and is justified by the fact that the present 2D computational results agree well with reported experimental work, as discussed in Section 3.

![Computational domain of the physical model](image)

Figure 1. Computational domain of the physical model

The diameter of the droplet \((D)\) is considered to be 2 mm, and based on this, the other dimensions of the computational domain are set. The diameter of the droplet \((D)\) is considered to be 2 mm, and based on this, the other dimensions of the computational domain are set. The side length of the square domain is considered to be \(L=10D\). The droplet is set to fall on the substrate from a distance of 0.01\(D\). The liquid droplet is considered to be water (fluid 1) with density \((\rho)\) and viscosity \((\mu)\) of 1000 kg/m\(^3\) and 0.001 Pas, respectively. The water droplet is surrounded by air (fluid 2) \((\rho=1.22 \text{ kg/m}^3, \mu=1.98 \times 10^{-5} \text{ Pas})\). The side boundaries are imposed with free-slip boundary conditions, whereas the top boundary of the domain is considered to be of constant pressure identical with the ambient pressure and no-slip boundary conditions are prescribed at the bottom. The effect of gravity is neglected as the size of the droplet is very small [21]. The initial velocity of the droplet is \(U=0.001 \text{ m/s}\) and the surrounding air is assumed to be stationary. The study puts emphasis on investigating the spreading behaviour changes with different wettability conditions of the wall combined with the interfacial tension of the droplet. Two specific wettability conditions were imposed on the surface: hydrophilic and hydrophobic with a contact angle \((\theta)\) of 78° and 150°, respectively. The influence of surface tension \((\sigma)\) with respect to imposed velocity is measured with a non-dimensional parameter called the Weber number \((\text{We} = \frac{\rho U^2 D}{\sigma})\) which was varied within a range of 0.001-0.0028.

2.2. Governing equations

The present study adopts the two-phase laminar flow level-set formalism for accurate capturing of interface based on finite element method. For this purpose, an implicit scalar function, the level-set
function, is defined to describe the minimum distance of any location from the interface as

\[
\phi(x,t) = \begin{cases} 
1 & \text{in the domain of fluid 1} \\
0 < \phi < 1 & \text{at the interface} \\
0 & \text{in the domain of fluid 2}
\end{cases}
\]

After defining the level-set function \( \phi(x,t) \), a generalised transport equation is solved to track the position of the interface throughout the domain as follows

\[
\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot \left( \lambda \nabla \phi - \phi \left( 1 - \phi \right) \nabla \phi \right),
\]

where \( t \) denotes time, \( u \) represents the velocity field, and \( \lambda \) is the diffusion coefficient, which is the product of the parameter controlling interface thickness \( (\epsilon_u) \) and a re-initialization parameter \( (\gamma) \).

Next, the level-set function is coupled with the velocity field in order to obtain the coupled Navier-Stokes equation, which can be expressed as

\[
\rho \left[ \frac{\partial u}{\partial t} + u \cdot \nabla u \right] = -\nabla P + \nabla \cdot \left[ \mu \left( \nabla u + \nabla u^T \right) \right] + \sigma \kappa \delta \left( r - r_i \right),
\]

where \( P \) is the pressure, \( \mu \) is the dynamic viscosity, \( \sigma \) is the fluid to fluid interfacial tension, \( \kappa \) is the curvature of the interface, \( \delta \left( r - r_i \right) \) is a delta distribution function that is zero everywhere except at the interface, and \( \hat{n} \) represents the normal direction to the drop surface. Equations (2) and (3) are solved with the continuity equation given by

\[
\nabla \cdot u = 0.
\]

3. NUMERICAL METHODOLOGY AND MODEL VALIDATION

A finite element method-based solver was employed to solve the governing equations (1)-(4). The mesh used for the present computational investigation is presented in Fig. 2, where the fluid-to-solid interacting zone is configured with very fine elements. Using the Galerkin weighted method and weak form transformation, the highly non-linear set of transport equations can be solved. The variables are solved iteratively up to a pre-set residual limit of \( 10^{-6} \). The present solver was tested for grid independence. Grid independent results were obtained for a grid with 59262 elements. For this grid, the variation of spreading length \( (L_s) \) shows a maximum 0.02% relative difference compared to the preceding grid system (with 47220 elements).

To test whether the solver accurately captures the interfacial dynamics it was used to solve the flow dynamics reported by Lin et al. [22] in their experimental study, where the impact of a droplet over a solid surface with different wettability conditions is extensively analysed. The flow conditions employed in the solver exactly replicated the experimental conditions of Lin et al. [22]. Figure 3 compares the results from the present solver with those reported by Lin et al. [22] and finds good agreement. Thus, the present solver is considered to be capable of capturing the interfacial dynamics.

4. RESULTS AND DISCUSSION

The present study investigates the spreading behaviour of droplet on a surface of a solid substrate. The main aim was to investigate how the spreading characteristics differ with varying wettability conditions of the surface and Weber number. Droplet interface morphology and droplet spreading length are determined for two different surface wettability conditions and a range of Weber numbers. The present study considers only two specific contact angles to represent the two wettability conditions: \( \theta = 150^\circ \) for hydrophobic wettability and \( \theta = 78^\circ \) for hydrophilic wettability.
The initiation of droplet-to-surface contact lags appreciably, as the droplet is yet to form the liquid-solid interface at the surface, whereas the hydrophobic surface tends to repel the interface from the liquid to solid attachment.

The spreading behaviour of droplet over a solid surface is highly influenced by the interfacial energy possessed by the droplet. Thus, the present study also explored the different scenarios considering the relative importance of inertia as well as surface tension force that can be expressed through the Weber number. Figure 6 describes the spreading characteristics of a droplet over a hydrophilic surface for three different Weber numbers. For $We=0.0028$, the droplet starts spreading at $\tau = 0.5$ (Fig. 6(a)) and subsequently the spreading length increases as the generated capillary wave pulls the interface laterally. The tip of the droplet shell (seen in Fig. 6(b)) becomes smaller under the effect of the capillary wave, and forms a crest in the middle, as can be observed at $\tau = 1.5$ (Fig. 6(c)). The wavy interface gradually becomes parallel to the solid substrate, with further spreading along the surface as seen at $\tau = 2.0$ (Fig. 6(d)). The trend remains similar when the Weber number decreases ($We=0.002, We=0.001$). However, it can clearly be seen in the figure that with the decrease in Weber number (increasing the surface tension), the spreading tendency increases. It is observed that at any given instant the spreading length is higher for lower values of Weber number. This is due to the fact that the interfacial force aids to the hydrophilicity of the surface and as a cumulative consequence the droplet interface spreads further over the surface. For a hydrophilic surface the droplet interface tends to move towards the surface; when the surface tension increases as $We$ decreases, the droplet interface again maintains the tension in the inward direction and retracts. Thus, as a cumulative consequence, the interface spreads further over the hydrophilic solid surface with decreasing Weber number. It is interesting to observe that at $We=0.001$, the droplet spreads the most compared to the other Weber numbers and strikes the boundary wall at $\tau = 2.0$ (Fig. 6(f)).

Droplet behaviour differs when the solid surface is hydrophobic (with all other conditions kept the
We = 0.0028  
(a) \( \tau = 0.5 \)
(b) \( \tau = 1.0 \)
(c) \( \tau = 1.5 \)
(d) \( \tau = 2.0 \)

\( We = 0.002 \)
(e) \( \tau = 0.5 \)
(f) \( \tau = 1.0 \)
(g) \( \tau = 1.5 \)
(h) \( \tau = 2.0 \)

\( We = 0.001 \)
(i) \( \tau = 0.5 \)
(j) \( \tau = 1.0 \)
(k) \( \tau = 1.5 \)
(l) \( \tau = 2.0 \)

Figure 6. Spreading characteristics of a droplet in terms of interfacial evolution shown at specified instants over a hydrophilic surface for three different We numbers

We = 0.0028  
(a) \( \tau = 1.0 \)
(b) \( \tau = 1.5 \)
(c) \( \tau = 2.0 \)
(d) \( \tau = 2.5 \)

\( We = 0.002 \)
(e) \( \tau = 1.0 \)
(f) \( \tau = 1.5 \)
(g) \( \tau = 2.0 \)
(h) \( \tau = 2.5 \)

\( We = 0.001 \)
(i) \( \tau = 1.0 \)
(j) \( \tau = 1.5 \)
(k) \( \tau = 2.0 \)
(l) \( \tau = 2.5 \)

Figure 7. Spreading characteristics of a droplet in terms of interfacial evolution shown at specified instants over a hydrophobic surface for three different We numbers

In a generalised framework it can be observed that for the hydrophobic surface the effect of the capillary wave propagating through the droplet interface is significantly suppressed by the repelling effect of the hydrophobic surface. As a consequence, the crest produced at the middle of the interface is not that remarkable, compared to hydrophilic surface. The concave interface formed in Figs. 7(c) & 7(f) quickly diminishes, forming a convex interface. It is well known that in case of a hydrophobic surface, the droplet interface is repelled from the surface and thus spreads less, whereas the increasing interfacial tension favours wider spreading of the liquid over the surface. In other words, two forces oppose to each other, meaning that the droplet interface exerts a resisting effect on the way of its expansion over the hydrophobic surface. Although the increasing interfacial tension due to decrease in Weber number provides favourable conditions for spreading, the repelling action of a hydrophobic surface also supresses expansion. Thus, at \( We = 0.0028 \) value, the droplet spreads gradually over the surface. However, with the decrease in We, the droplet spreads up to a critical limit, a point at which the interfacial tension prevails over the surface repelling of the hydrophobic surface and causes the droplet to retract, thus decreasing the length of spread. The retraction occurs as the hydrophobicity of the surface prevails over the interfacial tension. It can be observed from Fig. 7 that for \( We = 0.002 \), the droplet spreads up to \( \tau = 2.0 \), and then starts retracting, as can be observed at \( \tau = 2.5 \). The rebounding of droplet begins earlier, and with further decrease in We as it begins even earlier, at \( \tau = 2.0 \) for \( We = 0.001 \) (Fig. 7(k)).

The behaviour is summarised in Fig. 8. With the decrease in We the evolution of spreading length \( L_s \) increases as the increasing interfacial tension helps the droplet to spread more over the hydrophilic surface, as shown in Fig. 8(a). On the contrary, for
the hydrophobic surface shown in Fig. 8(b), the spreading length increases up to a critical limit and then starts decreasing as the droplet interface starts to retract with the decrease in Weber number. The initiation of retraction appears to occur earlier as Weber number decreases.

- Decreasing the Weber number results in larger spreading over the hydrophilic surface.
- In the case of the hydrophobic surface, spreading of the droplet increases with decreasing Weber number up to a critical limit, and then the droplet starts to retract. The initiation of retraction over the hydrophobic surface occurs earlier with the decrease in Weber number.

REFERENCES


