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Simulations of impinging droplets with surfactant-dependent dynamic contact angle

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ABSTRACT

An arbitrary Lagrangian–Eulerian (ALE) finite element scheme for computations of soluble surfactant droplet impingement on a horizontal surface is presented. The numerical scheme solves the time-dependent Navier–Stokes equations for the fluid flow, scalar convection–diffusion equation for the surfactant transport in the bulk phase, and simultaneously, surface evolution equations for the surfactants on the free surface and on the liquid–solid interface. The effects of surfactants on the flow dynamics are included into the model through the surface tension and surfactant-dependent dynamic contact angle. In particular, the dynamic contact angle (θ_d) of the droplet is defined as a function of the surfactant concentration at the contact line and the equilibrium contact angle (θ_e^0) of the clean surface using the nonlinear equation of state for surface tension. Further, the surface forces are included into the model as surface divergence of the surface stress tensor that allows to incorporate the Marangoni effects without calculating the surface gradient of the surfactant concentration on the free surface. In addition to a mesh convergence study and validation of the numerical results with experiments, the effects of adsorption and desorption surfactant coefficients on the flow dynamics in wetting, partially wetting and non-wetting droplets are studied in detail. It is observed that the effects of surfactants are more in wetting droplets than in the non-wetting droplets. Further, the presence of surfactants at the contact line reduces the equilibrium contact angle further when θ_e^0 is less than 90°, and increases it further when θ_e^0 is greater than 90°. Nevertheless, the presence of surfactants has no effect on the contact angle when $\theta_e^0 = 90°$. The numerical study clearly demonstrates that the surfactant-dependent contact angle has to be considered, in addition to the Marangoni effect, in order to study the flow dynamics and the equilibrium states of surfactant droplet impingement accurately. The proposed numerical scheme guarantees the conservation of fluid mass and of the surfactant mass accurately.

1. Introduction

Liquid droplets impinging on a solid substrate is encountered in many applications such as spray cooling, spray forming, spray coating, ink-jet printing, fuel injecting, etc. Apart form these applications, computations of impinging droplets are

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Nomenclature

Ψ	Mesh displacement
Γ	Boundary of Ω
Γ_1	Free surface
Γ_2	Liquid–solid interface
Ω	Computational domain
β	Slip number
β_ϵ	Slip coefficient
$\boldsymbol{\nu}_1$	Unit outward normal vector on Γ_1
$\boldsymbol{\nu}_2$	Unit outward normal vector on Γ_2
$\boldsymbol{\nu}_\zeta$	Co-normal vector at the contact line
$\boldsymbol{\tau}_{1,2}$	Scaled projection of $\boldsymbol{\nu}_1$ onto the plane $\Gamma_2(t)$
$\boldsymbol{\tau}_{2,2}$	Tangential vector on $\Gamma_2(t)$
$\hat{\Omega}$	Reference domain
$\hat{\sigma}$	Surface tension factor
$\mathcal{K}$	Sum of the principle curvatures
μ	Dynamic viscosity of fluid
$\otimes$	Tensor product
ρ	Density of fluid
σ_0^{ls}	Interfacial tension on the clean liquid–solid interface
σ_0^{sg}	Interfacial tension on the clean solid–gas interface
σ_0	Surface tension of a clean surface
σ_{ref}	Reference surface tension
θ_d	Dynamic contact angle
θ_e^0	Equilibrium contact angle on a clean surface
ζ	Contact line
∇_{Γ_1}	Surface gradient on Γ_1
∇_{Γ_2}	Surface gradient on Γ_2
$\mathcal{A}_t$	ALE mappings
$\mathbb{D}$	Deformation tensor
$\mathbb{I}$	Identity tensor
$\mathbb{P}_{\boldsymbol{\nu}_1}$	Projection operator onto the tangential plane of Γ_1
$\mathbb{S}$	Stress tensor
$\mathbb{S}_{\Gamma_1}$	Surface stress tensor
F_Y	Unbalanced Young force
C	Surfactant concentration in the bulk phase
C_Γ^∞	Maximum surface packing surfactant concentration
C_{Γ_1}	Surfactant concentration on the free surface
C_{Γ_2}	Surfactant concentration on the liquid–solid interface
$C_{\Gamma_{1,0}}$	Initial concentration on Γ_2
$C_{\Gamma_{1,0}}$	Initial surfactant concentration on Γ_1
D_1	Surface diffusion coefficient of C_{Γ_1}
D_2	Surface diffusion coefficient of C_{Γ_2}
D_c	Diffusion coefficient of bulk phase surfactant
E	Surfactant elasticity
K_1^a, K_2^a	Adsorption coefficients of surfactant on Γ_1, Γ_2
K_1^d, K_2^d	Desorption coefficients of surfactant on Γ_1, Γ_2
R	Ideal gas constant
T	Absolute temperature
U_τ	Tangential fluid velocity on the free surface/interface
$\mathbf{e}$	Unit vector in the direction opposite to gravitational force
$\mathbf{u}$	Fluid velocity
$\mathbf{v}$	Test function of velocity
$\mathbf{w}$	Domain velocity
c_0	Initial concentration of surfactants in the bulk phase
p	Pressure
q	Test function of pressure
u_{imp}	Impact speed
I	Given end time
L	Characteristic length
Q	Pressure space
U	Characteristic velocity
V	Velocity space
g	Gravitational constant
t	Time
Bi_1	Biot number of C_{Γ_1}
Bi_2	Biot number of C_{Γ_2}
Da	Damköhler number
Fr	Froude number
Pe_1	Peclet number of C_{Γ_1}
Pe_2	Peclet number of C_{Γ_2}
Pe_c	Peclet number
Re	Reynolds number
We	Weber number

also of a scientific interest for many researchers due to the challenges associated with it. Main challenges associated with computations of impinging droplets are to prescribe the boundary condition on the liquid–solid interface, especially at the moving contact line, and to incorporate the wetting effects, in particular, the inclusion of the contact angle into the model equations. In addition to these challenges, the presence of soluble surfactants in the droplet will complicate the model further.

Numerous studies on the choice of the boundary condition on the liquid–solid interface, especially in the vicinity of moving contact line, have been reported in the literature [8,10,12,32,41,52,53,60,64,71]. Using the usual no-slip boundary condition on the liquid–solid interface could induce an unbounded stress singularity at the moving contact line. This singularity is also called as kinematic paradox in the literature. Different types of slip boundary conditions have been proposed in the literature [12,41,71] to alleviate this singularity. Among all, the Navier-slip boundary condition is widely accepted, but it introduces the so-called slip coefficient. This unknown slip coefficient is also called as momentum transfer coefficient [36]. Even though a number of expressions have been proposed for the slip coefficient, it is often determined by comparing the computationally obtained wetting diameter with their corresponding experimental results [17]. Based on this approach, an expression for the slip coefficient has recently been proposed in [25] for computations of impinging droplets.