Supplementary information: Two-phase simulations of viscoplastic flow in superhydrophobic microchannels: interface stability, plug dynamics, and drag reduction

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I. OVERVIEW OF THE NUMERICAL WORKFLOW

This document provides a complete technical description of the computational framework used to simulate pressure-driven flow of a Bingham viscoplastic fluid over a superhydrophobic (SH) microchannel wall patterned with transverse grooves. The workflow, implemented in OpenFOAM, consists of several key stages. Initially, the two-dimensional finite computational domain is defined, and a structured mesh with local refinement is generated. Subsequently, the physical model and solver are configured; this includes setting up the two-phase Volume-of-Fluid (VOF) method, incorporating the regularized viscoplastic rheology, and defining the interfacial force model. The third stage involves specifying the boundary conditions at the inlet, outlet, and walls, as well as the initial conditions for the phase distribution. The solution is then executed via a transient simulation using the regularized constitutive model, continuing until a periodically developed flow state is achieved in the central grooves. Finally, the results are post-processed to extract the relevant flow fields, identify yielded and unyielded regions, and compute integral quantities such as the pressure drop and effective slip length.

II. GEOMETRY DEFINITION

A. Computational domain

The simulations were conducted in a two-dimensional domain representing a microchannel of height $2H$ and length $10L$, where L is the periodicity length of the grooves. The lower wall features ten identical, transversely oriented grooves, each characterized by a width $\hat{\delta}$ and depth $\hat{d}$. All the walls including the upper and bottom walls of the microchannel as well as the grooves' walls are smooth and imposes a no-slip condition. The half-height of the microchannel is denoted as reference length ($\hat{H}$), so two dimensionless parameters are introduced as the groove periodicity length $\ell = \hat{L}/\hat{H}$ and the slip area fraction $\varphi = \hat{\delta}/\hat{L}$. Additionally, the aspect ratio of the grooves is defined as $d = \hat{d}/\hat{\delta}$, reflecting the relative depth of the grooves.

B. Meshing strategy

A block-structured mesh was generated using OpenFOAM's `blockMesh` utility. A structured Cartesian grid was employed throughout the computational domain. For the streamwise direction, the number of cells per groove periodicity length was set to $n_x = 40$ for $\ell = 0.2$ and $n_x = 150$ for $\ell = 7$, ensuring adequate resolution of flow variations associated with the groove geometry. In the wall-normal direction, the main microchannel was discretized using $n_y = 400$ cells. Within the groove cavities, the wall-normal resolution $n_{y,g}$ varied depending on the groove depth d and groove periodicity length ℓ, ranging from 8 to 150 cells. Mesh stretching was applied in the wall-normal direction within the microchannel, with a refinement ratio of approximately 1/4 toward the solid walls to better resolve near-wall stress gradients. Inside the groove, additional refinement was applied normal to the liquid/air interface, with a refinement ratio of approximately 1/6 toward the interface to accurately capture interfacial dynamics. To further enhance resolution in critical regions, a rectangular zone encompassing the groove cavity and an adjacent layer of thickness $0.1H$ within the main microchannel was locally refined in both the streamwise and wall-normal directions using the refineMeshDict. This refinement procedure was applied twice, yielding a progressively finer mesh near the liquid/air interface and particularly near the groove edges, where large velocity and stress gradients are expected.

C. Dimensionless parameters

The flow is characterized by several dimensionless groups, defined as follows:

- Bingham number: $B = \hat{\tau}_0 \hat{H}/(\hat{\mu}_p \hat{U}_{\text{ave}})$
- Reynolds number: $R = \hat{\rho}_p \hat{U}_{\text{ave}} \hat{H}/\hat{\mu}_p$

Here, $\hat{H}$ is the channel half-height and $\hat{U}_{\text{ave}}$ is the average axial velocity. Moreover, $\hat{\mu}_p$ and $\hat{\tau}_0$ are the viscosity and yield stress of the viscoplastic fluid. The Capillary number is defined as $Ca = \hat{\mu}_p \hat{U}_{\text{ave}}/\sigma$ where the σ represents the surface tension coefficient between the air and viscoplastic fluid.

III. GOVERNING EQUATIONS AND CONSTITUTIVE MODEL

A. Two-phase flow formulation

The flow is governed by the incompressible Navier-Stokes equations for a mixture of two immiscible fluids: a viscoplastic liquid and air. The one-fluid formulation is employed, where the fluid properties are weighted by the volume fraction α, with $\alpha_1 = 1$ corresponding to the viscoplastic fluid and $\alpha_0 = 1$ to air. The continuity and momentum equations are given by:

$$\nabla \cdot \mathbf{U} = 0, \tag{1}$$

$$\left(\frac{\hat{\rho}}{\hat{\rho}_p}\right) R \left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U}\right) = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_s, \tag{2}$$

where $\mathbf{U} = U\mathbf{e}_x + V\mathbf{e}_y$ is the velocity field, P is the pressure and $\hat{\rho}_p$ is the reference density. The viscous stress tensor is denoted by $\boldsymbol{\tau}$, and the surface tension force is represented by $\mathbf{F}_s$, while the surface tension is modeled using the continuum surface force (CSF) model [1]. The fluid properties, including the mixture density $\hat{\rho}$ and viscosity $\hat{\mu}$, are calculated based on the volume fraction of each phase α_i, such that $\hat{\rho} = \alpha_0\hat{\rho}_a + \alpha_1\hat{\rho}_p$ and $\hat{\mu} = \alpha_0\hat{\mu}_a + \alpha_1\hat{\mu}_p$.

The subscripts p and a denote the viscoplastic and air phases, respectively.

B. Interface capturing

The evolution of the volume fraction α is governed by an advection equation, which includes an artificial compression term to maintain a sharp interface[2]:

$$\frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 \mathbf{U}) + \nabla \cdot [\alpha_1(1-\alpha_1)\mathbf{U}_c] = 0, \tag{3}$$

Here, $\mathbf{U}_c$ is a compression velocity field applied selectively in the interfacial region to counteract numerical diffusion.

C. Constitutive equations

The air phase is modeled as a Newtonian fluid, with its stress tensor given by:

$$\tau_a = \mu_a[\nabla\mathbf{U} + (\nabla\mathbf{U})^T], \tag{4}$$

where μ_a is the dynamic viscosity of air. The viscoplastic fluid is described by the Bingham model, regularized using the Papanastasiou method to facilitate numerical solution. The effective viscosity μ_{eff} is a function of the strain-rate magnitude $\dot{\gamma} = \sqrt{\frac{1}{2}\dot{\gamma}_{ij,p}\dot{\gamma}_{ij,p}}$:

$$\mu_g = 1 + \frac{B\,(1 - \exp{(-M\dot{\gamma})})}{\dot{\gamma}}, \tag{5}$$

where $\mu_g = \hat{\mu}_g/\hat{\mu}_p$ represents the dimensionless effective viscosity, and $M = \hat{m}\hat{U}_{ave}/\hat{H}$ is the regularization parameter. A value of $M = 10^3$ was selected based on a parametric study, providing a satisfactory compromise between numerical stability and accurate representation of the yield surface. Regions of the flow in which the strain-rate magnitude falls below $\dot{\gamma}_c$ re therefore classified as unyielded, while $\dot{\gamma}_c$ obtained by solving the implicit relation [3, 4]:

$$\dot{\gamma}_c = \frac{1}{M}\,\ln(\frac{B}{\dot{\gamma}_c}), \tag{6}$$

IV. NUMERICAL METHODOLOGY AND SOLVER CONFIGURATION

A. Solver details

The simulations were performed using the transient, incompressible, two-phase solver `multiphaseInterFoam` from the OpenFOAM framework. The solution algorithm follows a sequentially coupled approach. First, the volume fraction transport equation (Equation (3)) is solved to update the phase distribution. The mixture properties (density and viscosity) are then recalculated based on the new volume fraction field. Next, the momentum predictor step is executed. Pressure-velocity coupling is enforced using the PIMPLE algorithm, which merges aspects of the PISO and SIMPLE methods. This involves solving a pressure correction equation, correcting the mass fluxes and velocities, and iterating for 3 correction steps within each time step to ensure strong coupling. This sequence repeats until the convergence criteria for the time step are satisfied.

B. Discretization schemes

The spatial and temporal discretization schemes were prescribed through the OpenFOAM case dictionaries. Time integration was performed using a first-order implicit Euler scheme, which ensures numerical robustness for the transient simulations considered. Spatial gradients were discretized using a Gauss linear scheme, providing second-order accuracy on structured meshes. For the convective terms, different divergence schemes were employed depending on the transported quantity. The momentum convection term was discretized using a Gauss upwind scheme, prioritizing numerical stability in regions with sharp velocity gradients. The transport of the volume fraction field was handled using a Gauss van Leer scheme, which is a bounded, second-order total variation diminishing (TVD) scheme that effectively preserves interface sharpness while minimizing numerical diffusion. The additional interface compression flux was discretized using a Gauss linear scheme. Viscous stress divergence terms were discretized using a Gauss linear scheme. Laplacian terms were discretized using a second-order Gauss linear corrected scheme to account for mesh non-orthogonality. Face values of interpolated quantities were obtained using linear interpolation. Normal gradients at cell faces were evaluated using a corrected snGrad scheme to ensure second-order accuracy on non-orthogonal meshes.

C. Solver settings and tolerances

The iterative linear solvers and convergence criteria were specified in the `fvSolution` dictionary. The pressure correction equations (`pcorr` and `pcorrFinal`) were solved using a Preconditioned Conjugate Gradient (PCG) solver with a Diagonal Incomplete Cholesky (DIC) preconditioner and a Gauss–Seidel smoother. For the intermediate pressure correction (`pcorr`), an absolute tolerance of 1×10^{-8} and zero relative tolerance were imposed, with a maximum of 1000 iterations. The final pressure correction (`pcorrFinal`) employed an absolute tolerance of 1×10^{-7} with zero relative tolerance.

The modified pressure variable p_{rgh} was also solved using the PCG solver with DIC preconditioning. An absolute tolerance of 1×10^{-7} and a relative tolerance of 0.05 were applied for the intermediate iterations, while the final pressure solve (`p_rghFinal`) enforced a zero relative tolerance, a maximum of 20 iterations, and two V-cycles to ensure consistent convergence.

The velocity field was solved using a `smoothSolver` with a symmetric Gauss–Seidel smoother. An absolute tolerance of 1×10^{-7} and a relative tolerance of 0.01 were applied for the intermediate velocity solution, while the final velocity solve enforced the same absolute tolerance with zero relative tolerance.

The transport of the volume fraction fields was handled using a compressive algebraic interface-capturing approach. Two outer correction steps ($n_\alpha = 2$) with four sub-cycles per time step ($n_{\alpha,\mathrm{sub}} = 4$) were applied for each phase, and an interface compression factor of $c_\alpha = 2$ was used to maintain a sharp liquid/air interface.

Pressure–velocity coupling was achieved using the PIMPLE algorithm with one outer corrector and three inner pressure correctors, without non-orthogonal corrections. The momentum predictor was disabled to enhance numerical stability in the strongly coupled two-phase viscoplastic flow simulations.

D. Under-relaxation factors

To promote numerical stability, under-relaxation factors were applied. The pressure field was relaxed with a factor of 0.1, while the velocity equation was relaxed with factors of 0.3.

E. Time-step control

A variable time-stepping method was employed, with the time step dynamically adjusted to maintain a maximum Courant number of $Co_{\max} = 10^{-2}$. This constraint is essential for maintaining stability in the interface-capturing calculation.

V. BOUNDARY AND INITIAL CONDITIONS

A. Boundary conditions

The boundary conditions applied in the simulations are summarized as follows. At the inlet, a fixed velocity profile obtained from an analytical model of Poiseuille–Bingham flow in the same microchannel without grooves was imposed. This profile corresponds to the target average velocity $\hat{U}_{\mathrm{ave}}$ and Bingham number B [5, 6]. A zero-gradient condition was prescribed for pressure, and a fixed value of $\alpha = 1$ (pure viscoplastic fluid) was imposed for the volume fraction. At the outlet, a fixed total pressure of zero (atmospheric reference) was applied, together with zero-gradient conditions for velocity and volume fraction. All solid walls, including the upper channel wall, the lower wall ridges, and the groove walls and bottom, were treated as impermeable no-slip boundaries for velocity, with zero-gradient conditions imposed for both pressure and volume fraction. It is important to note that the shear-free condition at the liquid/air interface was not imposed explicitly as a boundary condition. Instead, it emerges naturally from the solution of the two-phase system, driven by the large viscosity and density contrasts between the phases ($\hat{\mu}_a/\hat{\mu}_p \sim 10^{-3}$ and $\hat{\rho}_a/\hat{\rho}_p \sim 10^{-3}$), in conjunction with the CSF formulation.

B. Initial conditions

The simulations were initialized using a prescribed velocity field and pressure distribution. The initial velocity field was set equal to the analytical Poiseuille–Bingham velocity profile corresponding to the target average velocity $\hat{U}_{\text{ave}}$ and Bingham number B in a smooth microchannel without grooves [5, 6]. The initial pressure field p was set to the reference pressure, consistent with the outlet pressure condition. The groove cavities were initially filled with air, while the remainder of the computational domain was filled with the viscoplastic fluid. This phase distribution was initialized using OpenFOAM's `setFields` utility.

VI. SIMULATION PIPELINE

The simulation pipeline began with pre-processing steps, including the generation of the computational mesh using `blockMesh` and initialization of the phase field using `setFields`. The transient solver `multiphaseInterFoam` was then executed to advance the two-phase viscoplastic flow in time. Each simulation was continued until the flow within the central grooves (typically from the fifth groove onward) reached a repeatable, quasi-periodic state, indicating that inlet transients had dissipated. Convergence was monitored by tracking the residuals of the velocity components and pressure at each time step, ensuring that the velocity residuals fell below 1×10^{-8}. In addition to residual-based criteria, physical convergence was verified by monitoring the axial velocity profiles at the center of each groove and the morphology of the liquid/air interface. Once both the velocity profiles and interface shape became time-invariant, the solution was considered converged and representative of the final steady-state flow regime.

VII. POST-PROCESSING METHODOLOGY

Upon reaching a statistically periodic state, the flow fields were sampled for post-processing and analysis. The OpenFOAM output data were imported into MATLAB scripts, which were used to generate all contour plots and line profiles presented in this work. The identification of yielded and unyielded regions was performed as a post-processing step by flagging computational cells in which the local strain-rate magnitude $\dot{\gamma}$ fell below the critical value $\dot{\gamma}_c$ defined in Equation (6). Moreover, all reported output quantities were computed using the governing definitions provided in the manuscript and evaluated within the MATLAB framework. Throughout this study, the liquid/air interface position and deformation were determined from the $\alpha_1 = 0.5$ isocontour, which was adopted as the nominal interface location.

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