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COMPUTATIONAL MODELING OF FREE-SURFACE FLOW PERTINENT TO DROPLET IMPACT ON A POROUS SUBSTRATE

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ABSTRACT
The report is aimed at formulating and validating the computational model for the isothermal two-phase flow with free-surfaces incorporating porous medium. The flow configuration consists of the liquid droplet impacting on and simultaneously spreading over and within a porous substrate. The interface capturing methodology implemented in the open-source software OpenFOAM® based on the volume-of-fluid (VOF) model in the framework of Computational Fluid Dynamics (CFD) is extended to incorporate the flow within the porous medium. The potential of the model is evaluated by contrasting the results of numerical simulations to the existing experimental results.
Keywords: free-surface flow, computational modeling**,** porous medium, volume-of-fluid

1. INTRODUCTION
The phenomenon of droplet collision is a challenging physical problem, rich in fluid dynamics, requiring insight which may enable improvements in many technical, environmental and industrial fields. Detailed studies of its dynamics were not possible before high-speed digital cameras could be used for photography and powerful computers for numerical computations. A number of influencing factors may affect the outcome: the droplet may not be of a perfect spherical shape, the impacting target may be a dry or partially wetted, flat or curved, normal or inclined, hard or deformable porous substrate, the liquid may be non-Newtonian, miscible, etc. [1]. Droplet impact onto a porous surface is a fluid dynamical phenomenon present in everyday life and encountered in various engineering applications. It is common in ink-jet printing or in composite processing, where the air in the porous medium is displaced by a polymeric fluid. Recent development in medicine in the field of the needle-free vaccine delivery emphasizes the importance of studying the liquid penetrating into the porous medium [2]. Due to the complexity of the porous network, theoretical solutions provide only limited information about the dynamics of the flow and experimental observations cannot fully reveal the behavior within the porous medium. In this study the computational model for interface capturing is formulated and the procedure is applied to compute droplet impact on a porous surface. The computational model based on the well-known volume of fluid (VOF) method [3] is extended and the combined model is formulated including both the external flow for the spreading and the flow of the absorbed fluid in the porous substrate. The numerical model is validated by comparing the computational results with the existing experimental results from [4].

2. GOVERNING EQUATIONS AND NUMERICAL DETAILS
The two parameters characterizing the porous substrate are its porosity and permeability. Porosity represents a measure of the volume of the pore spaces in the material and is defined as the fraction of the volume of the pores over the total volume of the porous material $\varepsilon = V_p / V$. Permeability is used to quantify the ability of the fluid to flow through the porous material and is defined by Darcy's law for the flow in the porous material $\langle U \rangle = -(K/\mu)(\Delta p / L)$, where the symbol $\langle\ \rangle$ denotes the averaged or superficial velocity. The mathematical formulation of the isothermal free-surface flow

includes the interface capturing methodology extended to incorporate the flow within the porous substrate. The momentum equation inside the porous material is extended to include the Darcy-Forchheimer flow resistance [5]. The details of the interface capturing model are given in [6]. The governing transport equations are the conservation of mass, phase fraction and momentum

$$\nabla \cdot \langle \mathbf{U} \rangle = 0 \qquad \text{... (1)}$$

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot \left(\langle \mathbf{U} \rangle \gamma \right) + \nabla \cdot \left[\langle \mathbf{U}_c \rangle \gamma (1-\gamma) \right] = 0 \qquad \text{... (2)}$$

$$\frac{\partial \left(\rho \langle \mathbf{U} \rangle \right)}{\partial t} + \frac{1}{\varepsilon} \nabla \cdot \left(\rho \langle \mathbf{U} \rangle \langle \mathbf{U} \rangle \right) = -\nabla \langle p_d \rangle - \varepsilon \mathbf{g} \cdot \mathbf{x} \nabla \rho + \nabla \langle \mathbf{T} \rangle + \varepsilon \sigma \kappa \nabla \gamma - \frac{\varepsilon \mu}{K} \langle \mathbf{U} \rangle \qquad \text{... (3)}$$

with $\langle p_d \rangle = \varepsilon p_d$ being the averaged macroscopic modified pressure, the averaged stress tensor $\langle \mathbf{T} \rangle = \mu \nabla \left(\langle \mathbf{U} \rangle + \langle \mathbf{U} \rangle^T \right)$ corresponds to the definition of the averaged velocity, and porosity and permeability are assumed constant. The other symbols are the same as defined in [6]. The fluids are treated as a homogeneous mixture of gas and liquid, the properties of which are determined as weighted averages based on the phase fraction distribution γ. The effects of the surface tension are accounted for by the Continuum Surface Force model (CSF) [7] neglecting spatial variation of surface tension. The computations were carried out using OpenFOAM®, an open-source CFD software distributed by the OpenFOAM Foundation [8]. The phase fraction γ, although a discontinuous function in reality, changes smoothly over the interface in the model. The smearing of steep gradients is suppressed by the additional counter-gradient transport term in the phase fraction equation acting against the numerical diffusion. The flow equations are solved in a solution procedure incorporating an iteration loop in every time step, solving iteratively the fluid motion. Fluid properties are updated after each time step and are determined by the phase fraction distribution. The numerical procedure incorporates a cell-center-based finite volume approximation of the transport equations. The transient terms are evaluated using the Euler implicit scheme and the spatial convective derivatives terms are integrated over cell face surfaces with the cell face values of dependent variables determined by the Van Leer flux limiter. The pressure is coupled with velocity by the Pressure Implicit with Splitting of Operators (PISO) algorithm. The computational domain for the combined model, shown in Fig. 1, is a two-dimensional axisymmetric slice including both the external and the porous region.

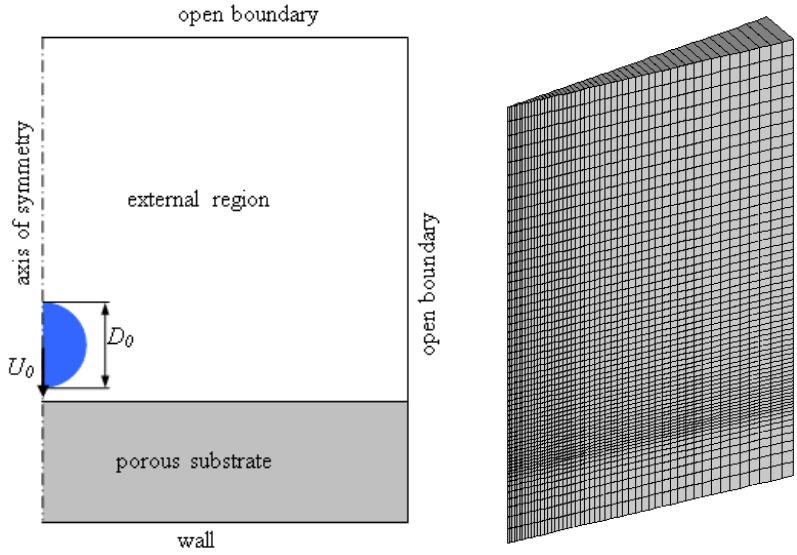

Figure 1. Initial case configuration (left) and computational mesh (right, every fourth line shown) for the combined model.

For a better resolution the mesh is graded, with dimensions in the vertical plane of $4D_0 \times 6D_0$ based on the droplet initial diameter with the total of 48000 cells, 8000 belonging to the porous region.

Simulations are initialized by prescribing the phase fraction distribution defining the shape of the drop and setting the initial impact velocity. The boundary conditions for the combined model include the no-slip wall boundary at the bottom and open boundaries at the top and to the right side with the prescribed total pressure and a combination of inlet and outlet conditions for velocity.

3. RESULTS

A review of the available literature has revealed that drop impact on fibrous media was not extensively studied, most studies not providing exact values for the permeability, and the experiments being mostly performed on sessile droplets. The assessment of both computational models is performed using the experimental data for drop impact on the ceramic porous substrate from [4] where the liquid used is n-heptane (C_7H_{16}) with the impact velocity U_0 = 0.93 m/s and the droplet diameter D_0 = 1.5 mm, corresponding to Reynolds and Weber numbers of Re = 2300 and We = 43, respectively. In order to assess the predictive capabilities of the combined model the computationally obtained spreading ratio and the change of the lamella height at the axis of symmetry in time are compared to the experimental results. In addition, the decrease of the lamella volume above the porous surface is computed, which determines the absorbed liquid volume. Fig. 2 and Fig. 3 show the comparison of the computed spreading ratio and the change of the lamella height at the axis of symmetry in time with the existing experimental results [4], and Fig. 4 shows the computed residual volume of the lamella over the porous substrate during spreading. The lamella height and volume are normalized by the drop initial diameter and volume.

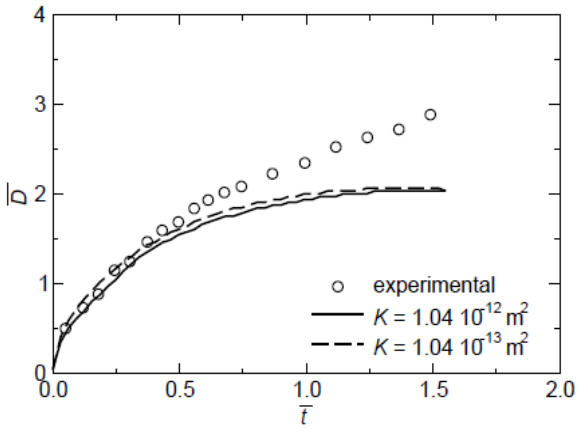

Figure 2. Droplet spreading ratio on the porous surface

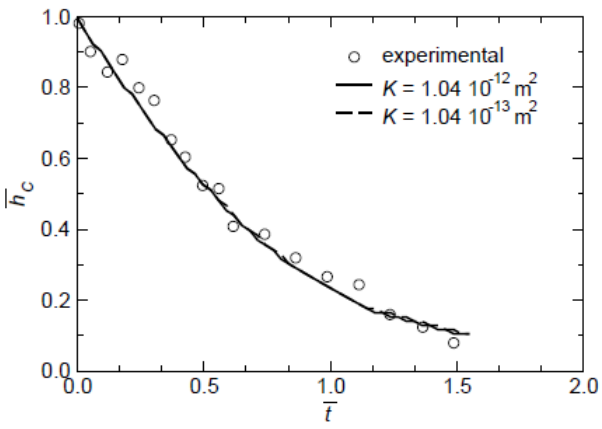

Figure 3. Dimensionless lamella height at the symmetry axis

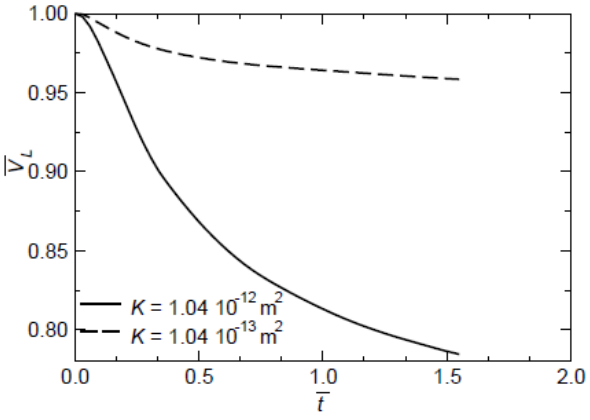

Figure 4. Dimensionless lamella volume above the porous surface

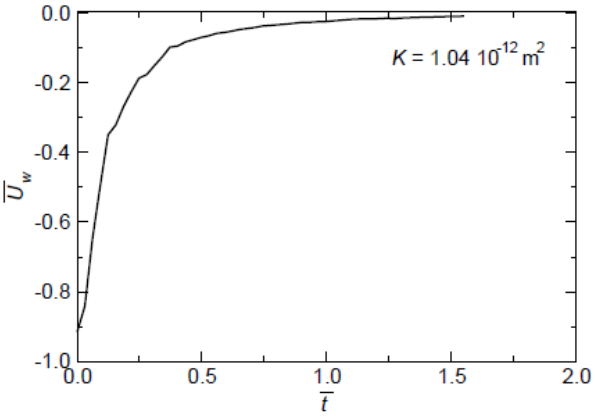

Figure 5. Dimensionless mean velocity at the porous surface

The numerical results of the combined model show a good agreement with the experimental data, particularly in the first inertia dominated period of the flow. The permeability of the porous medium has negligible effects on the spreading ratio and the lamella height during the initial spreading phase, indicating the fact that the time scale for the liquid absorption is much larger than that for the spreading. The computationally determined residual liquid volume above the porous surface shows a non-linear dependence with time. As expected, the model predicts greater liquid volumes above the porous surface for the substrate with lower permeability, due to the lower absorbed liquid volume. Fig. 5. shows the computed mean velocity normalized by U_0, which, as expected, is decreasing since there is no other driving force for the absorption except inertia and the velocity of the penetration decreases in time.

4. SUMMARY AND CONCLUSIONS

The computational model for isothermal two-phase flow with free-surfaces in the porous medium is formulated and validated. The model includes the interface capturing methodology based on the volume-of-fluid (VOF) model extended to capture the effects of the flow within the porous medium. The model validation is performed using numerical simulations of the flow generated by the impact of a liquid droplet on the porous substrate. The potential of the computational model is evaluated by comparing the numerically obtained results with the existing experimental results. The computed flow configuration indicated by the droplet spreading ratio and the lamella height show a good agreement with the previously reported results. Moreover the lamella volume and the mean liquid velocity at the porous surface are computed numerically. The computational procedure based on the numerical model demonstrates good predictive capabilities by reproducing correctly the characteristics of the studied flow. The computational model can be used to obtain temporal development of the flow and the spatial distribution of the free-surface enabling a detailed insight into the flow, as well as the analysis of other similar two-phase flows with free-surfaces.

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