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A smoothed particle hydrodynamics model for droplet and film flow on smooth and rough fracture surfaces

J. Kordilla [a,*], A.M. Tartakovsky [b], T. Geyer [a]

[a] Geoscientific Centre, University of Göttingen, Goldschmidstr. 3, D-37073 Göttingen, Germany
[b] Computational Mathematics Group, Pacific Northwest National Laboratory, Richland, WA 99352, USA

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ABSTRACT

Flow on fracture surfaces has been identified by many authors as an important flow process in unsaturated fractured rock formations. Given the complexity of flow dynamics on such small scales, robust numerical methods have to be employed in order to capture the highly dynamic interfaces and flow intermittency. In this work we use a three-dimensional multiphase Smoothed Particle Hydrodynamics (SPH) model to simulate surface tension dominated flow on smooth fracture surfaces. We model droplet and film flow over a wide range of contact angles and Reynolds numbers encountered in such flows on rock surfaces. We validate our model via comparison with existing empirical and semi-analytical solutions for droplet flow. We use the SPH model to investigate the occurrence of adsorbed trailing films left behind droplets under various flow conditions and its importance for the flow dynamics when films and droplets coexist. It is shown that flow velocities are higher on prewetted surfaces covered by a thin film which is qualitatively attributed to the enhanced dynamic wetting and dewetting at the trailing and advancing contact lines. Finally, we demonstrate that the SPH model can be used to study flow on rough surfaces.

1. Introduction

Understanding the physics of fast flow through unsaturated fractured rocks is important for management of groundwater resources and prediction of repository performance in hard rock regions [1,2]. The uncertainties range from process understanding at local scale to that of hydraulic understanding of regional fault zones [3]. Simulation of unsaturated flow in hard rocks represents a challenge due to highly non-linear free-surface flow dynamics and the complexity of interactions between flow in a fracture and the surrounding matrix. Hard rock formations contain fractures and other discontinuities with varying spatial parameters including orientation, density and aperture distributions [2]. Volumetric flow rates of water in unsaturated fractures may differ by several orders of magnitude from flow rates through the porous rock matrix. In sites where the rock matrix has a small permeability, fractures may provide the primary pathways for percolation of water to the phreatic zone [4]. In this case, classical modeling approaches [5,6] for unsaturated flow in porous media may not be accurate for flow in fractured rocks.

Recent laboratory experiments of Tokunaga and Wan [7] and Tokunaga et al. [8] have shown that film flow contributes significantly to the overall unsaturated flow in fractured rocks. Depending on the matric potential, i.e., the saturation of the matrix, films with thickness up to 70 μm and average flow velocity of $3 \cdot 10^{-7}$ m/s may develop on fracture surfaces providing an efficient preferential pathway for laminar flow. Even faster flow velocities on fracture surfaces may develop due to the presence of droplets [9,10], continuous rivulets [11–15] and falling (turbulent) films [16]. As noted by Doe [9] and Ghezzehei [16] these flow regimes may coexist with adsorbed films, however their influence on the faster flow regimes such as droplets has not been investigated by these authors and is also part of this work.

Flow rates during transitions between droplets, rivulets and falling films can range significantly in magnitude, and have been investigated by Ghezzehei [16] using an energy minimization principle. The approach is partially based on the findings of Podgorski et al. [17]. The authors investigated droplet flow on inclined surfaces and proposed a dimensionless linear scaling law to quantify flow velocities and provide a general framework and a unified dimensionless description of such flow processes. In order to apply the scaling to arbitrary fluid-substrate systems Ghezzehei [16] introduced a dimensionless scaling parameter. In this study, we employ this scaling law in a quantitative study of droplet flow on dry and wet fracture surfaces.

Given the complexity of the small-scale flow dynamics and the heterogenous nature of fractured rock surfaces, numerical models provide a significant addition to laboratory experiments and analytical solutions to investigate these systems. Models have to resolve the highly dynamic fluid interfaces as well as boundary geometries.

* Corresponding author.
E-mail address: jkordil@gwdg.de (J. Kordilla).

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Traditional grid-based methods, such as Finite-Element or Volume of Fluid [18,19] methods, in general require complex and computationally demanding interface tracking schemes. Furthermore, these methods have to rely on empirical boundary conditions specifying dynamic receding and advancing contact angles as a function of velocity. Lagrangian particle methods offer a versatile treatment of multiphase flows in domains with a complex geometry. In particle methods, there is no need for front-tracking algorithms to detect a moving interface as it moves with the particles. In addition particle methods are rigorously Galileian invariant as particle interactions only depend on relative differences in positions and velocities of the interacting particles. Furthermore, particle methods exactly conserve mass, energy and momentum due to antisymmetric particle–particle forces. Depending on the form of forces acting between particles, particle methods can model fluid flow on different spatio-temporal scales.

Molecular Dynamics (MD) is able to accurately model multiphase fluid flow on a molecular scale but modeling flow in a reasonably-sized porous domain or fracture is far out of reach of modern MD codes, even for state-of the-art High-Performance computers.

Smoothed Particle Hydrodynamics (SPH) [20,21] can be seen as upscaled formulations of MD in which particles represent fluid volumes and forces acting between particles of the same fluid phase are obtained from a meshless discetization of the Navier–Stokes equations [22]. Due to the similarity to MD, the surface tension and static and dynamic contact angles can be modeled via molecular-like pair-wise interaction forces [23]. Making these forces "soft", i.e., creating forces that have a finite magnitude for small (and zero) distances between a pair of particles, allows the SPH multiphase model to simulate flow on hydrodynamics time and length scales. A critical review of various numerical methods for multiphase flows in porous and fractured media can be found in Meakin and Tartakovsky [24]. Application of SPH for modeling flow in porous media has been demonstrated by, authors [25–28].

In this work we use a SPH model to study free-surface fluid flow on smooth and rough wide aperture fractures, i.e., flow bounded by a single fracture surface. This SPH model has been used before to study multiphase and free surface flows [23,29,30,27], but has not been rigorously validated for three-dimensional free-surface flow dominated by capillary forces. We demonstrate that the SPH method of Tartakovsky and Meakin [23] can be applied to model dynamics of droplets on dry surfaces. Our simulations show how wetted surfaces naturally arise from droplet wetting dynamics and demonstrate the effect of prewetted surfaces on droplet flow.

The objectives of this work are: (1) the verification of the SPH model with existing empirical and semi-analytical solutions; (2) the investigation of droplet wetting behavior on initially dry surfaces for a wide range of wetting conditions; and (3) the study of transient droplet flow on fracture surfaces covered by adsorbed films using the SPH model. To ensure numerical accuracy of the SPH simulations, the effect of resolution on static contact angles is investigated. Contact angle hysteresis for droplets in a critical state, i.e., at the verge of movement, is simulated and compared to laboratory data of ElSherbini and Jacobi [31,32]. Transient droplet flow is verified using the dimensionless linear scaling of Podgorski et al. [17]. The formation of adsorbed films emitted from droplets on initially dry fracture surfaces and their influence on droplet flow is investigated. The effect of surface roughness on flow velocities is demonstrated.

2. Method

In the following we give a brief description of the SPH method and the governing equations. More detailed derivations and approximations involved in the SPH method can be found for example in [33,23].

To derive a SPH discretization of the Navier–Stokes equations, one can start with the definition of the Dirac function, δ,

$$f(\mathbf{r}) = \int_{\Omega} f(\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}')d\mathbf{r}', \tag{1}$$

where $f(\mathbf{r})$ is a continuous function defined on a domain Ω and $\mathbf{r}$ is the position vector. In SPH, for computational reasons, the δ function is replaced with a smooth, bell-shaped kernel function W [33] that produces a smoothed approximation $\langle f(\mathbf{r})\rangle$ of $f(\mathbf{r})$:

$$\langle f(\mathbf{r})\rangle = \int_{\Omega} f(\mathbf{r}')W(|\mathbf{r}-\mathbf{r}'|,h)d\mathbf{r}'. \tag{2}$$

For the sake of simplicity we drop the angular brackets denoting the approximation in the following. The kernel $W(|\mathbf{r}-\mathbf{r}'|,h)$ satisfies the normalization condition

$$\int_{\Omega} W(|\mathbf{r}-\mathbf{r}'|,h)d\mathbf{r}' = 1 \tag{3}$$

and has a compact support h such that $W(r,h) = 0$ for $r > h$, where $r = |\mathbf{r}|$. In the generalized limit of $h \to 0$, the following condition is satisfied:

$$\lim_{h\to 0} W(|\mathbf{r}-\mathbf{r}'|,h) = \delta(\mathbf{r}-\mathbf{r}'). \tag{4}$$

We use a fourth-order weighting function W [34]:

$$W(|\mathbf{r}|,h) = \alpha_k \begin{cases} \left(3-\frac{3|\mathbf{r}|}{h}\right)^5 - 6\left(2-\frac{3|\mathbf{r}|}{h}\right)^5 + 15\left(1-\frac{3|\mathbf{r}|}{h}\right)^5 & 0 \leqslant |\mathbf{r}| < \frac{1}{3}h \\ \left(3-\frac{3|\mathbf{r}|}{h}\right)^5 - 6\left(2-\frac{3|\mathbf{r}|}{h}\right)^5 & \frac{1}{3}h \leqslant |\mathbf{r}| < \frac{2}{3}h \\ \left(3-\frac{3|\mathbf{r}|}{h}\right)^5 & \frac{2}{3}h \leqslant |\mathbf{r}| < \frac{2}{3}h \\ 0 & |\mathbf{r}| > h \end{cases} \tag{5}$$

where $\alpha_k = 81/(359\pi h^3)$.

Eq. (2) can be approximated as

$$f(\mathbf{r}) = \sum_{j=1}^{N} f(\mathbf{r}_j)W(|\mathbf{r}-\mathbf{r}_j|,h)\Delta V_j, \tag{6}$$

where the domain space is discretized with a set of N particles. If $f(\mathbf{r})$ is a scalar or vector property of a fluid (e.g., fluid density or velocity), then we replace the finite volume ΔV_j by m_j/ρ_j (m_j and ρ_j are the mass and mass density of a fluid carried by particle j) and obtain a general SPH approximation for f and its gradient in terms of the values f at points $\mathbf{r_j}, f_j = f(\mathbf{r_j})$,

$$f(\mathbf{r}) = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} W(|\mathbf{r}-\mathbf{r}_j|,h), \tag{7}$$

and

$$\nabla f(\mathbf{r}) = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} \nabla W(|\mathbf{r}-\mathbf{r}_j|,h), \tag{8}$$

where $\nabla W(|\mathbf{r}-\mathbf{r}_j|,h)$ is computed analytically from Eq. (5).

Flow of each fluid phase is governed by the continuity equation,

$$\frac{d\rho}{dt} = -\rho(\nabla\cdot\mathbf{v}) \tag{9}$$

and the momentum conservation equation

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho}\nabla P + \frac{\mu}{\rho}\nabla^2\mathbf{v} + \mathbf{g}, \tag{10}$$

subject to the Young–Laplace boundary conditions at the fluid–fluid interface