Simulation of film and droplet flow on wide aperture fractures using Smoothed Particle Hydrodynamics

Jannes Kordilla, Tobias Geyer
Applied Geosciences
Georg-August-Universität Göttingen
Göttingen, Germany
jkordil@gwdg.de

Alexandre Tartakovsky
Computational Science and Mathematics Division
Pacific Northwest National Laboratory
Richland, USA
alexandre.tartakovsky@pnnl.gov

Abstract—Simulation of flow in fractured porous media represents a challenge due to the highly non-linear dynamics of fluid-air interfaces. Here we present small-scale flow simulations on wide aperture fractures using a modified three-dimensional multiphase SPH model [1]. The model is enhanced to include the effects of random thermal noise and able to reproduce a wide range of wetting conditions and Reynolds numbers encountered in laboratory experiments using pairwise fluid-fluid and solid-fluid interaction forces. Static and transient flow dynamics are compared to empirical and semianalytical solutions: (1) Droplets in a critical state are in agreement with laboratory experiments using the fluctuation-dissipation theorem and its effect on dynamics of droplets in a critical state is investigated. (2) Transient flow dynamics on dry surfaces are validated using the dimensionless relationships established by [3] and compared to (4) dynamics on prewetted surfaces where flow velocities are shown to be nearly tripled. Finally we establish flow regimes and occurrence of trailing films on initially dry fracture surfaces based on dimensionless scaling parameters and Reynolds numbers.

I. INTRODUCTION

Aquifers are the largest water reservoirs for continental freshwater. Groundwater recharge depends on the geometrical and hydraulic properties of the vadose zone (rock formations between surface and water table) where pore space is only partially filled with water. The underlying saturated zone, delineated by the water table, may reach depths of several hundred meters and therefore is coupled to the hydrodynamic state of the unsaturated zone. Quantification of recharge and water travel times through the unsaturated zone are of importance for understanding of large-scale hydraulic behavior, transport of contaminants, management of groundwater resources and nuclear waste repositories ([4],[5]).

The large heterogeneity of the hydraulic parameter field found in fractured geological media represents a challenge for numerical modeling of flow and transport, especially in the unsaturated zone, where high flow intermittency ([6],[7],[8]), preferential pathways ([9],[10],[11]), and complex interaction of porous matrix and fractures have to be considered ([12],[13]). Most macro-scale effective unsaturated flow models underestimate flow velocities and travel time distributions on local scale even though they might be adequate to simulate catchment scale dynamics.

Small scale flow dynamics in fractures are governed by the complex interplay of body and surface forces resulting in several flow regimes such as absorbed films ([14]), droplets ([3],[15],[7]), rivulets ([16],[17]) and traveling liquid waves which all contribute to the rapid movement of water through the unsaturated zone and interaction with the porous matrix system.

Here we want to present simulations of flow in fractured media in order to gain a deeper understanding of the complex flow dynamics and show the versatility of Smoothed Particle Hydrodynamics in this context.

II. METHOD

In the following we give a brief description of our model and the governing equations. Detailed derivations and approximations involved in the SPH method can be found, for example, in ([18],[19]). We use an SPH discretization of the Navier-Stokes equations following [1]:

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left( \frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} \right) \nabla W_i(|\mathbf{r}_{ij}|, h)$$

$$+ \eta_{ij} + g + m_i \sum_{j=1}^{N} \mathbf{F}_{ij}$$

where \(\mathbf{v}\) is the particle velocity, \(t\) is the time, \(P\) and \(\rho\) denote pressure and density, \(m\) is mass of particle \(i\) and \(g\) is the gravitational acceleration. Following [20] a fourth-order weighting function \(W_i\) is employed where the support of \(W_i\) is set to \(h = 1.0\) and all particles are assumed to have the same mass, \(m_i = 1.0\) for computationally efficiency. All variables in the SPH model are given in consistent model units. The viscosity term \(\eta_{ij}\) is given by [21] as

$$\eta_{ij} = 2\mu \frac{\mathbf{v}_{ij}}{\rho_i \rho_j r_{ij}} \frac{\partial W}{\partial r_{ij}}.$$  (2)
We model surface tension using a particle-particle interaction force \( \sum_{i=1}^{N} \mathbf{F}_{ij} \) [20]. The force consists of two superimposed cubic spline kernels \( W_1(|\mathbf{r}_i - \mathbf{r}_j|, h_1) \) and \( W_2(|\mathbf{r}_i - \mathbf{r}_j|, h_2) \) (22):

\[
\mathbf{F}_{ij} = \begin{cases} 
  s_{ij} [AW_1(r, h_1) + BW_2(r, h_2)] & |\mathbf{r}_i - \mathbf{r}_j| \leq h \\
  0 & |\mathbf{r}_i - \mathbf{r}_j| > h,
\end{cases}
\]

(3)
such that a smooth and continuous function with a short-range repulsive and long-range attractive part is created (see Fig. 1). The following parameters are used: \( A = 2.0, h_1 = 0.8, B = -1.0 \) and \( h_2 = 1.0 \) with \( W_1(|\mathbf{r}_i - \mathbf{r}_j| > 0.8, h_1) = 0 \). The strength of the force is independently controlled for fluid-fluid and fluid-solid interactions by the parameter \( s_{ij} \) which assumes values \( s_{fs} \) (fluid-solid) and \( s_{ff} \) (fluid-fluid).

We obtain the density from the general field approximation

\[
\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_i - \mathbf{r}_j|, h)
\]

(4) and close the equation system by a van der Waals type equation of state:

\[
P = \frac{\rho_0 h T}{1 - \rho \frac{a}{m} \rho^2}
\]

(5)

where \( k_0 \) is the Boltzmann constant, \( T \) is the temperature and \( a \) and \( b \) are the van der Waals constants. Values for the constants are \( k_0 T = 1.6, a = 3.0 \) and \( b = 1/3 \).

III. MODEL CALIBRATION

A. Surface Tension

In order to determine the surface tension we prescribe a value for the fluid-fluid interaction force \( s_{ff} \) and obtain the pressure through the Young-Laplace law:

\[
\sigma_{sph} = \frac{R_{eq}}{2} \Delta P,
\]

(6)

where \( \sigma_{sph} \) is the surface tension, \( R_{eq} \) is the equilibrated drop radius and \( \Delta P \) is the pressure difference between drop and airphase. We do not discretize the airphase, therefore the pressure difference \( \Delta P \) is equal to the drop pressure \( P_0 \). As the interaction forces do not contribute to the pressure obtained from the equation of state we evaluate \( P_0 \) using the Virial theorem as shown by [1] and [23]:

\[
P_0 = \frac{1}{2 \rho V} \sum_i \sum_j \mathbf{r}_{ij} f_{ij} = \frac{1}{8 \pi \rho_{sph}} \sum_i \sum_j \mathbf{r}_{ij} f_{ij},
\]

(7)

where \( f_{ij} = m_i dV_i / dt \) and \( d = 3 \) for a three-dimensional system. As the particles within distance \( 1h \) from the surface suffer from a slight boundary deficiency we set \( r_{virial} = R_{eq} - h \). The first summation is carried out using all particles within distance \( r_{virial} \) from the center of the droplet, while the second sums over all particles. To exclude the boundary effect, we set \( r_{virial} = R_{eq} - h \). For a given value of \( s_{sf} = 0.05 \) we obtained a surface tension of \( \sigma_{sph} = 0.25 \) which is used for all the shown simulations in this work.

B. Static Contact Angles

Given the fluid-fluid interaction force \( s_{ff} \) and and the shape of the interaction potential the static contact angles depend on the solid-fluid interaction force \( s_{sf} \). We studied the dependence of the contact angle on the magnitude of \( s_{sf} \) as well as the model resolution by slowly equilibrating drops on a smooth surface. For static conditions we relate our units using the dimensionless Bond number:

\[
Bo = \frac{\rho g V^{2/3}}{\sigma},
\]

(8)

where \( V \) is the volume of a droplet. Given the average model density \( \rho_{sph} = 39.2 \), surface tension \( \sigma_{sph} = 0.25 \) a droplet with \( Bo = 1 \) is simulated for different resolutions, i.e. varying radii \( R_{eq} = 1.77 h \) (902 particles) to \( R_{eq} = 5.85 h \) (77993 particles) with volumes \( V = 23.3 - 839.0 h \) by adjusting the gravitation acceleration to \( g_{sph} = 7.82 \times 10^{-4} - 7.17 \times 10^{-4} \). Droplets are slowly placed on the surface by gradually decreasing the gravitational acceleration and \( s_{sf} \).

Simulations yield contact angles which are practically independent of resolution over the whole range of solid-fluid interaction forces from \( s_{sf} = 0.001 \) to \( 0.05 \). Simulations in this work use interaction forces between \( s_{sf} = 0.01 \) to \( 0.05 \) corresponding to static contact angles of \( 110^\circ \) to \( 25^\circ \).
IV. CRITICAL CONTACT ANGLES

In addition to the static contact angle measurements we conducted numerical experiments for droplets in a critical state, i.e. at the verge of movement. Experimental data of [2] and [24] suggests a dimensionless relationship between Bond number and critical contact angles independent of the fluid-solid configuration.

A drop under dynamics conditions can be characterized by an advancing contact angle $\theta_A$ perpendicular to the direction of motion and a receding contact angle $\theta_R$ at the droplet tail. Here the Bond number is defined as:

$$ Bo' = \frac{\rho g (2R)^2}{\sigma} \sin(\alpha), $$

where $\alpha$ is the inclination angle of the surface measured from the horizontal. Contact angles around the perimeter of the drop range from $\theta_{min}$ to $\theta_{max}$ during the transition from static conditions to movement. However, as shown by [2] for several fluid-substrate combinations and Bond numbers ranging from 0.0 to 3.0 the maximum angle $\theta_{max}/\theta_A \approx 1.0$ such that $\theta_{max} \approx \theta_A$. Furthermore the minimum contact angles $\theta_{min}$ is shown to match the receding contact angle $\theta_R$ through the transition, therefore we restrict our measurements of the critical contact angles to $\theta_R$ and $\theta_A$. Based on their laboratory experiments [24] propose the following quadratic non-linear relationship between $\theta_{min}/\theta_A$ and $Bo'$:

$$ \frac{\theta_R}{\theta_A} = \frac{\theta_{min}}{\theta_A} = 0.01Bo'^2 - 0.155Bo' + 0.97. \quad (10) $$

Our numerical experiments consist of several fluid-substrate configuration with static contact angles ranging from 60° to 110° which yield results in the range of $Bo'$ from 0.0 to 3.0 similar to the laboratory experiments. Drop sizes vary between $R_{eq} = 1.77$ and 5.85 which corresponds to $Bo' = 0.14 - 2.8$ for a critical state. Gravitational acceleration is set to $g_{sph} = 0.000164$ with droplets being carefully equilibrated on the surface. We then slowly decrease the inclination angle by one degree every 500 time steps to give drops enough time to adjust and to be able to determine the exact onset of movement and measure the contact angles (see Fig. 2).

The simulation results are consistent with the experiments of [2] (see Fig. 3). We observe a slight deviation for higher values of $Bo'$. As this is within the data variance of our experiments and the laboratory experiments we cannot conclude if a numerical insufficiency is responsible for the deviation.

V. TRANSIENT DROPLET DYNAMICS

Despite the complexity involved in hydrodynamics of transient droplets ( [25], [26], [27], [28]) simpler dimensionless relationships help to calibrate the model to a variety of wetting conditions encountered in highly heterogeneous systems such as fractured media. Here we presents our results of transient droplet dynamics ( [29]). To verify droplet dynamics over a wide range of static contact angles, Bond numbers and Capillary numbers we conducted extensive numerical experiments and applied the proposed dimensionless scaling law of [3]:

$$ Ca \sim Bo\sin(\alpha) - \Delta \theta, \quad (11) $$

The Capillary number is defined as

$$ Ca = \frac{\mu v}{\sigma} \quad (12) $$

![Fig. 2. Droplets in a critical state before the onset of motion. Droplet radius is 4.82 μm ($Bo = 1.02$) and static contact angles range from 60° to 110°.](image)

![Fig. 3. Droplets in a critical state right before the onset of motion. A critical state for large values of Bo’ can only be obtained from droplets with high values of the solid-fluid interaction strength, i.e. low static contact angles.](image)
where $v$ is the droplet velocity and $\Delta \theta$ is a perimeter-averaged projection factor of surface tension. A useful extension of the scaling has been proposed by [30] to apply results to various fluid-substrate configuration:

$$Ca = \gamma \, Bo \sin(\alpha) - \Delta \theta$$  \hspace{1cm} (13)

where $\gamma$ is a dimensionless scaling parameter unique for every fluid-substrate combination.

### A. Dry Surfaces

The simulation domain has sizes $x = 128 \, h$, $y = 64 \, h$ and $z = 16 \, h$ which corresponds to 45.7x22.8x5.7 mm in SI units. Droplet sizes are varied in the range of 0.14 to 1.5 in terms of the Bond number (nine droplet radii from 1.77 $h$ to 5.85 $h$), while surface inclinations range from 10$^\circ$ to 90$^\circ$ yielding 81 values $Bo \sin(\alpha)$ and $Ca$ values for every static contact angle $\theta_0$. The viscosity assumes three values ($\mu = 0.01$, 0.03, 0.1) to cover the wide range of Reynolds numbers observed in water-rock systems.

Droplet velocities are measured when the maximum velocity is reached by evaluating the change of droplet front position in time $\Delta x / \Delta t$ where $\Delta t$ is chosen over a linear interval. The results show that the linear relationship holds over wide ranges of viscosities and static contact angles (see Fig. 4), however, a few exceptions have to be considered when the assumptions for the scaling are violated: (1) Droplets whose shape deviates strongly from the rounded or cornered shape (i.e. assume a rivulet shape with strong tailing) slow down due

![Fig. 4. Example of results for static contact angles $\theta_0 = 60^\circ$ and $\theta_0 = 80^\circ$ and three viscosities. Scaling parameters are obtained using only droplets with shapes that do not strongly deviate from the rounded or cornered shape (i.e. below the dashed lines).](image)

![Fig. 5. Development of trailing films on initially dry surfaces for varying strength of the solid-fluid interaction strength $s_{sf}$. Shown surfaces are tilted at an angle of 90$^\circ$.](image)
Fig. 6. Maximum Reynolds numbers and flow regimes for all investigated static contact angles (dry and prewetted conditions). Trailing films appear more pronounced at higher Re and $s_{sf}$ values.

Prewetted surfaces yield velocities which can be increased by a factor of three indicating the importance of adsorbed films and adequate integration of such effects into the SPH model when studying flow in fractured media.

VI. RANDOM THERMAL FLUCTUATIONS

The effect of random noise introduced to particle systems has been demonstrated for example by [31] (DPD) and [32] and [33] (SDPD). Here we want to investigate the influence of thermal noise added to the momentum equation via the fluctuation-dissipation theorem [34]:

$$\frac{dv_i}{dt} = \sum_j \frac{1}{m_j} \sigma_{ij} d\overline{W} e_{ij} \Delta t^{-1/2}$$ (15)

where $d\overline{W}$ is the traceless symmetric part of a matrix of independent random numbers with variance one and mean zero and $e_{ij}$ is a normalized vector. $\sigma_{ij}$ can be obtained through the fluctuation-dissipation theorem by comparing the irreversible part of the dynamics:

$$\sigma_{ij} = \sqrt{-8T^* \mu \left( \frac{1}{\rho_i \rho_j} \right) \frac{1}{r_{ij}} \partial W / \partial r_{ij}}$$ (16)

The added random forces act as a thermostat to keep the whole system at a constant kinetic temperature, i.e. energy dissipation through viscous forces until the system freezes is prevented. Fig. 7 shows the development of the kinetic energy of an infinite domain of size $x = y = z = 4$ h after introducing

Fig. 7. Kinetic energy of the periodic system for temperatures $T^* = 1.0 \times 10^{-6}, 2.0 \times 10^{-6}, 3.0 \times 10^{-6}, 4.0 \times 10^{-6}, 5.0 \times 10^{-6}$ (from bottom to top).
the thermal energy $T^*$. All fluid properties are the same as described previously.

After reaching a constant kinetic energy we determine the diffusion coefficient of the system by means of the positional variance $\sigma^2_r$ over time (see Figs. 8 and 9) defined as:

$$D = \left[ \frac{1}{N} \sum_{i=1}^{N} (r_1(t) - r_1(t_0))^2 \right] / \Delta t$$ (17)

We use the dimensionless Schmidt number $S_c$

$$S_c = \frac{\mu}{\rho D}$$ (18)

to relate the diffusion coefficients in model units to real units. Schmidt numbers for water at average subsurface temperatures of 6 °C to 15 °C range from about 700 to 1500 which corresponds to a range of $T^*$ from $2.0 \times 10^{-6}$ to $5.0 \times 10^{-6}$. In order to investigate the effect of additional thermal noise on the droplet dynamics we introduce a constant temperature of $T^* = 3.0 \times 10^{-6}$ to the simulations as shown in section IV to determine critical contact angles with added random forces.

Results indicate a slightly better fit to the data of [2], especially for lower static contact angles, (see Fig. 10). However, given the the relatively high data variance results should be interpreted with caution. The current simulations run at a rather coarse resolution, considering the length scales associated with thermal fluctuations, i.e. the mean free path of molecules. Nevertheless, surface interactions might be affected by thermal fluctuations when using higher resolutions which is scope of future research.

VII. CONCLUSION

We applied a three-dimensional free-surface SPH model including the effects of surface tension and thermal fluctuation to simulate droplet flow on smooth surfaces. It is shown that our model can capture the behavior of droplets over a wide range of fluid-solid configurations. Critical contact angles are shown to reproduce laboratory experiments and transient droplet dynamics on dry surfaces follow a linear scaling. We investigated the limitations of the SPH model, e.g. the occurrence of trailing films for static contact angles below 60° and strong deviations in droplet shape. Prewetted surfaces are shown to increase droplet velocities and display the importance of such effects for percolation of water through fractured media. Finally we have investigated the influence of random thermal fluctuations added to the momentum equations via the fluctuation-dissipation theorem and show that critical contact angles are possibly affected.

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Fig. 10. Critical contact angles with random thermal fluctuations.

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