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

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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 solidfluid 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 of [2]. (2) Well-defined random thermal noise is introduced via the fluctuation-dissipation theorem and its effect on dynamics of droplets in a critical state is investigated. (3) 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 occurence 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]:

$$\frac{d\mathbf{v}_{i}}{dt} = -\sum_{j=1}^{N} m_{j} \left(\frac{P_{j}}{\rho_{j}^{2}} + \frac{P_{i}}{\rho_{i}^{2}} \right) \boldsymbol{\nabla} W_{i}(|\mathbf{r}_{ij}|, h)
+ \boldsymbol{\eta}_{ij} + \mathbf{g} + m_{i} \sum_{j=1}^{N} \mathbf{F}_{ij}$$
(1)

where **v** is the particle velocity, t is the time, P and ρ 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 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 η_{ij} is given by [21] as

$$\boldsymbol{\eta}_{ij} = 2\mu \frac{\mathbf{v}_{ij}}{\rho_i \rho_j r_{ij}} \frac{\partial W}{\partial r_{ij}}.$$
(2)



Fig. 1. Interaction potential.

We model surface tension using a particle-particle interaction force $\sum_{j=1}^{N} \mathbf{F}_{ij}$ [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]):

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

$$\rho_i = \sum_{j=1}^N m_j W(|\boldsymbol{r}_i - \boldsymbol{r}_j|, h) \tag{4}$$

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

$$P = \frac{\rho \frac{k_b}{m}T}{1 - \rho \frac{b}{m}} - \frac{a}{m}\rho^2 \tag{5}$$

where k_b is the Boltzmann constant, T is the temperature and a and b are the van der Waals constants. Values for the constants are $k_bT = 1.6$, 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:

$$\sigma_{sph} = \frac{R_{eq}}{2} \Delta P, \tag{6}$$

where σ_{sph} is the surface tension, R_{eq} is the equilibrated drop radius and ΔP is the pressure difference between drop and airphase. We do not discretize the airphase, therefore the pressure difference ΔP 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]:

$$P_0 = \frac{1}{2dV} \sum_i \sum_j \mathbf{r}_{ij} \mathbf{f}_{ij} = \frac{1}{8r_{virial}^3} \sum_i \sum_j \mathbf{r}_{ij} \mathbf{f}_{ij}, \quad (7)$$

where $\mathbf{f}_{ij} = m_i d\mathbf{v}_i/dt$ 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:

$$Bo = \frac{\rho g V^{2/3}}{\sigma},\tag{8}$$

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 $\mathbf{g}_{sph} = 7.82 \times 10^{-4} - 7.17 \times 10^{-4}$. 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° to 25° .



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

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 θ_A perpendicular to the direction of motion and a receding contact angle θ_R at the droplet tail. Here the Bond number is defined as:

$$Bo' = \frac{\rho g(2R)^2}{\sigma} \sin(\alpha), \tag{9}$$

where α is the inclination angle of the surface measured from the horizontal. Contact angles around the perimeter of the drop range from θ_{min} to θ_{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 θ_{min} is shown to match the receding contact angle θ_R through the transition, therefore we restrict our measurements of the critical contact angles to θ_R and θ_A . Based on their laboratory experiments [24] propose the following quadratic non-linear relationship between θ_{min}/θ_A and Bo':

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

Our numerical experiments consist of several fluid-subtrate 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.



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.

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 heterogenous systems such as fractured media. Here we presents our results of transient droplet dynamics on dry and wet surfaces ([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]:

$$Ca \sim Bo\sin(\alpha) - \Delta_{\theta},$$
 (11)

The Capillary number is defined as

$$Ca = \mu v / \sigma \tag{12}$$



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).

where v is the droplet velocity and Δ_{θ} 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:

$$Ca = \gamma \ Bo\sin(\alpha) - \Delta_{\theta} \tag{13}$$

where γ 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° to 90° yielding 81 values Bo $\cdot \sin(\alpha)$ and Ca values for every static contact angle θ_0 . The viscosity assumes three values ($\mu_{sph} = 0.01, 0.03, 0.1$) 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 Δt 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. 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°.



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.

to increased surface area interaction and (2) for high values of s_{sf} , i.e. low static contact angles, droplet volumes are not constant as they leave behind trailing films (see Fig. 5)

B. Prewetted Surfaces

In order to investigate the effect of prewetted surfaces on droplet dynamics and the scaling we set up a second simulation with particles covering the surface as a flat film. The film thickness is chosen equal to the thickness of trailing films for each strength of s_{sf} under the assumption that this represents the maximum fluid capacity for the given fluidsubstrate system. At the chosen model resolution continuous trailing films are stable for $s_{sf} = 0.04$ and 0.05. Films applied to systems with higher static contact angles results in a Marangoni-like breakup of films and are not considered here.

The film thickness varies between 0.3-0.5 h corresponding to 107-178 μ m. This value is in the right order of magnitude ([12], [14], 2-70 μ m and [7], 0.9-40 μ m), however, it is obvious that higher SPH resolutions are need to fully resolve these length scales.

Fig. 6 gives a comprehensive overview of the results obtained from the simulations in terms of maximum Reynolds numbers (with respect to each static contact angle and all droplet radii) and flow regimes encountered, where the Reynolds number is defined as:

$$Re = \frac{\rho \ v \ V^{(1/3)}}{\mu}.$$
 (14)

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]:

$$\frac{d\mathbf{v}_{i}}{dt} = \sum_{j} \frac{1}{m_{j}} \sigma_{ij} d\overline{\overline{\mathcal{W}}} \mathbf{e}_{ij} \Delta t^{-1/2}$$
(15)

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

$$\sigma_{ij} = \sqrt{-8T^*\mu\left(\frac{1}{\rho_i\rho_j}\right)\frac{1}{r_{ij}}\frac{\partial W}{\partial r_{ij}}}$$
(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 $T^* = 1.0 \times 10^{-6}$, 2.0×10^{-6} , 3.0×10^{-6} , 4.0×10^{-6} , 5.0×10^{-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 σ_r^2 over time (see Figs. 8 and 9) defined as:

$$D = \left[\frac{1}{N}\sum_{i=1}^{N} \left(\mathbf{r}_{i}(t) - \mathbf{r}_{i}(t_{0})\right)^{2}\right] / \Delta t$$
(17)

We use the dimensionless Schmidt number S_c

$$S_c = \frac{\mu}{\rho D} \tag{18}$$

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 2.0×10^{-6} to 5.0×10^{-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 occurence 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. 8. Development of the positional variance $\sigma_{\mathbf{r}}^2$ over time. The variance has been measured after reaching a thermostatic equilibrium at time step t = 210. The diffusion coefficient is determined using the linear data beginning at time step t = 260.



Fig. 9. Diffusion coefficient D obtained from the simulations. Droplet simulations use $T^* = 3.0 \times 10^{-6}$ which corresponds to a Schmidt number of 840 for water at approx. 10 °C.

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

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