PRF # 57371-DNI9
Project title: Controlling particle migration using geometry and hydrodynamics
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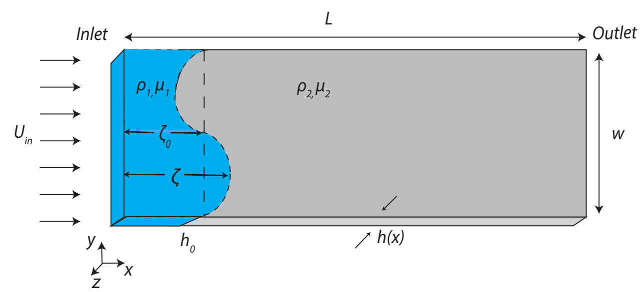


Figure 1: Top view of a rectilinear Hele-Shaw cell. Depth gradient exists in the flow-wise direction. The lubrication approximation ensures that the governing equations are identical to Darcy flow in a porous medium with effective permeability $k(x) = \frac{1}{12}[h(x)]^2$.

Summary of Progress: The PI and his team developed a mathematical model of the stability of the interface between two fluids in a Hele-Shaw cell (see geometry and notation in Fig. 1). This model, featuring two clear immiscible fluids separated by a surface-tension-laden interface, represents a building block in understanding the effects of geometry on multiphase subsurface flows.

Specifically, we extended the classical Saffman–Taylor stability criterion for immiscible displacements to capture the effect of geometric variation in the flow-wise direction. Here, the variation is modeled by the changing depth (the "small" dimension), $h(x)$, of a Hele-Shaw cell. For a linear taper $h(x) = h_0 + \alpha x$, we found the linear growth rate $\dot{\lambda}$ satisfies

$$(1+M)\left(\frac{\dot{\lambda} h_0}{U} + 3\alpha\right) = \left(1 - M + \frac{2\alpha\cos\theta_c}{Ca}\right) h_0 k - \frac{k^3[h\big(\zeta_0(t)\big)]^2 h_0}{Ca}, \tag{1}$$

as a function of the two fluids' viscosity ratio M, the channel depth at the inlet h_0, the depth gradient $\alpha = [h(x) - h_0]/x$, the contact angle θ_c, the wavenumber k of the initial unstable disturbance, and the capillary number $Ca = 12\mu_2 U/\gamma$, where γ is the surface tension. Equation (1) quantifies the growth rate for viscous fingering in the presence of geometric variations. It allows us to determine a critical capillary number by letting $\dot{\lambda} = 0$:

$$Ca_c = \frac{2\alpha\cos\theta_c - k^2[h(\zeta_0)]^2}{3(1+M)\frac{\alpha}{kh_0} + (M-1)}. \tag{2}$$

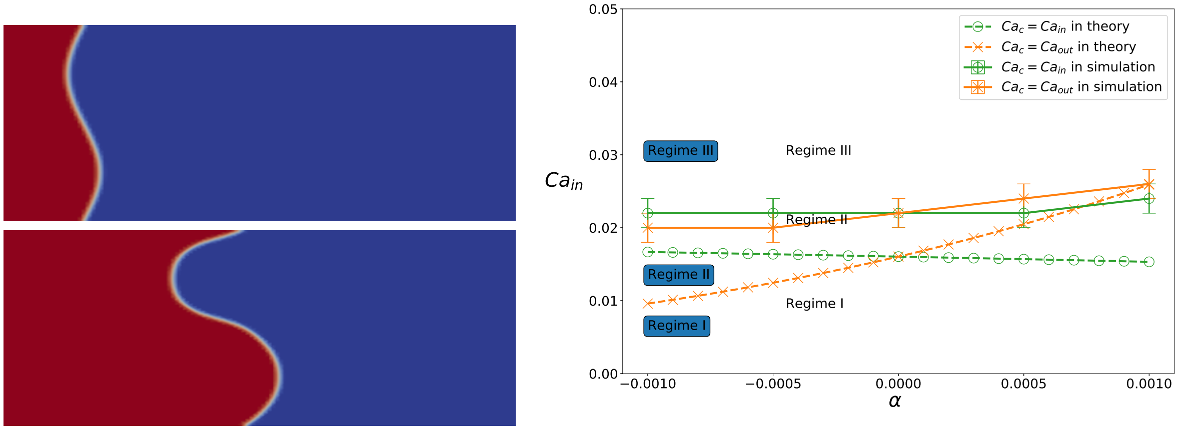
From Eq. (2) we can determine whether a fluid–fluid displacement in a tapered geometry is stable or unstable. For applications in secondary oil recovery it is desirable to push through a stable interface, though water displacing oil in a fixed-depth gap is Saffman–Taylor unstable.

An important consequence of geometric variations is that the local capillary number varies along the flow direction. Then, on the basis of Eq. (2), we can divide the (in)stability scenarios of the interface into three regimes for a given Hele-Shaw cell, based on the difference between Ca_c and the Ca_{local}. If $Ca_c > \min Ca_{local}$, then the interface is always stable: Regime I; if $\min Ca_{local} < Ca_c < \max Ca_{local}$, then the interface could change its stability type as it propagates through the narrow conduit: Regime II; if $Ca_c < \max Ca_{local}$, then the interface is always unstable: Regime III. $\min Ca_{local}$ and $\max Ca_{local}$ are Ca values at the inlet or outlet, depending on the sign of α.

Next, we set out to validate our mathematical prediction by high-fidelity numerical simulations. We built a fully 3D computational model of the flow scenario from in Fig. 1 using the OpenFOAM platform. We used the InterFoam solver, which is based on the volume-of-fluid method, to evolve the fluid-phase-field and capture surface tension effects. Adding an interface-compressing term in the continuity equation improved the sharpness of the interface for immiscible displacements. Figure 2(a) shows an example simulation in the always unstable Regime III.

Carrying out a computational parametric study on Purdue University's Brown Computing Cluster, on which we purchased computational nodes through the generous support of this ACS PRF award, we were able to map out the three-regime diagram numerically. In general, simulations (based on a fully 3D model capturing all physics of the problem) support and justify our linear-stability-based regime diagram, as shown in Fig. 2(b). This analysis provides concrete guidelines on how to control interfacial instabilities using geometric variations.

Next we set out to extend these results to particle-laden multiphase flows, as initially proposed. In this case, we consider the displaced fluid to be a clear liquid, while the displacing fluid is a particle-laden mixture (dense suspension). The interface between the two fluid is no longer a sharp surface-tension-laden boundary but it is rather a region over which the particle concentration varies sharply from constant values ahead and behind the front. A mathematical analysis of this problem is still ongoing.



(a) Perturbed unstable fluid–fluid interface at $t = 0$s (top) and $t = 50$s (bottom) in Regime III.

(b) Stability diagram with geometric variations. Dashed lines are theoretical division of three regimes. Solid lines separate the numerical regimes.

Figure 2: The evolution of viscous fingering under geometric variations in the flow-wise direction: (a) dynamic simulation in OpenFOAM and (b) stability diagram in the presence of a geometric variation captured by the depth gradient α. Ca_{in} and Ca_{out} represent the inlet and outlet capillary numbers, respectively.

We set up a numerical model for particle migration in a suspension at low Reynolds number in the presence of a geometric variation. We focused on non-Brownian shear-dominated suspensions, where kinetic collisions are negligible and frictional effects play a dominant role. Under these circumstances, irreversible phenomena like particle diffusion and migration develop, requiring anisotropic stress models to describe the suspension rheology. On a continuum level, reduced-order models like the suspension balance model (SBM) or the diffusive flux model are commonly used to predict particle migration phenomena. We proposed, instead, a new method based on the two-fluid model (TFM), where both the phases are considered as interpenetrating continua. Specifically, we showed (see Fig. 3) that when an anisotropic stress analogous to that used in the SBM is added to the equilibrium equations for the particle phase, the TFM is able to predict particle migration. Unlike the SBM, the TFM does not require the assumptions of a steady suspension velocity of vanishing Reynolds number. Our numerical simulations were performed using the twoPhaseEulerFoam solver in OpenFOAM.

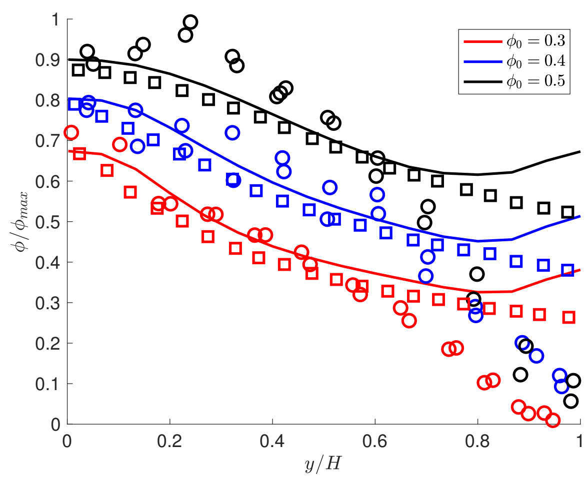


Figure 3: Particle migration in a dense suspension in a slot of height H at steady state. Solid curve: this work; ○: Lyon and Leal (1998), experiment; □: Miller and Morris (2005), SBM simulation. $\phi(y)$ is the particle volume fraction with ϕ_0 the inlet one.

Career Impact: This research is the dissertation topic of the PI's first PhD student at Purdue, Daihui Lu, who's developing theoretical and numerical models of viscous fingering under geometric variations. Dr. Federico Municchi, a postdoctoral scholar not funded by the award but collaborating with us, has been providing guidance on the OpenFOAM development and gaining mentorship experience. The ACS PRF award supported Daihui Lu's presentations on this topic at the American Physical Society's Prairie Section meeting in 2017 and at the U.S. National Congress on Theoretical and Applied Mechanics in 2018, affording her significant professional development opportunities. Three undergraduates gained research experience under this research project: Zihao Lin and Zoë S. Penko (Summer Research Fellows), and Pranay Nagrani (S.N. Bose Fellow). Zihao Lin was mentored by Daihui Lu on the Saffman–Taylor problem described above, Zoë Penko was mentored by the PI on free-surface flows in shaped channels/cracks, and Pranay Nagrani was mentored by Federico Munnichi on OpenFOAM simulations of two-fluid models of dense particulate suspensions in the presence of geometric variations. All three are considering graduate studies in engineering.