Electronic Supplementary Material (ESI) for Soft Matter.

Using evaporation to control capillary instabilities in micro-systems
Supplementary Information

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3D model and lattice-Boltzmann simulations

We model the liquid and gas phases as a binary fluid, in which each phase is labelled using a phase field $\phi(x, y, z, t)$. The phase field varies continuously between the two volume phases, which are separated by a diffuse interface. In the same spirit, all other hydrodynamic variables, namely the density, ρ, viscosity, η, chemical potential, μ, pressure, p, and velocity, $\mathbf{v}$, vary smoothly across the interface.

In equilibrium, the configuration of the two-phase system is determined by the Helmholtz free-energy functional [**? ?**]

$$\mathcal{F} = \int_V \left(F_\mathrm{b} + \frac{\kappa}{2} |\boldsymbol{\nabla}\phi|^2 \right) \mathrm{d}V + \int_S (\kappa_\mathrm{s}\phi_\mathrm{s}) \mathrm{d}S, \tag{1}$$

where V is the total volume of the binary fluid and S is the surface of the confining solid walls. The first term in the volume integral corresponds to the bulk free-energy density

$$F_\mathrm{b} = \frac{\rho}{3} \log \rho + \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4, \tag{2}$$

which contains an ideal gas term to ensure incompressibility, where we have introduced the local mass density of the fluid, ρ, and a double-well potential term in which a and b are model parameters. With this choice of F_b, phase separation occurs if $a < 0$ and $b > 0$. The resulting two equilibrium phases have bulk phase field values $\phi_\mathrm{b} = \pm\sqrt{-a/b}$. Here we fix $b = -a$ and take $\phi_\mathrm{b} = -1$ to be the gas phase and $\phi_\mathrm{b} = +1$ to represent the liquid. The square-gradient term in equation (1) represents the energy cost of spatial variations of ϕ across the system. In equilibrium, it leads to the formation of a diffuse interface of typical width $\xi = \sqrt{-2\kappa/a}$ and surface tension $\gamma = \sqrt{-8\kappa a/9}$.

The surface integral in equation (1) models the wetting properties of the binary fluid, where ϕ_s represents the value of the phase field at the solid surfaces. In equilibrium, this term leads to the boundary condition

$$\partial_n \phi_\mathrm{s} = -\frac{\kappa_\mathrm{s}}{\kappa}, \tag{3}$$

where n indicates the coordinate normal to the solid surface. The parameter κ_s can be tuned to control the contact angle of the fluid-fluid interface with the solid, θ_e, through the relation

$$\cos\theta_\mathrm{e} = \frac{1}{2}\left[(1+\Omega)^{3/2} - (1-\Omega)^{3/2}\right], \tag{4}$$

where $\Omega = \kappa_\mathrm{s}\sqrt{1/\kappa a}$.

The phase-field approach can be used to model a phase change by introducing an imbalance in the chemical potential of the binary fluid, defined as

$$\mu \equiv \frac{\delta\mathcal{F}}{\delta\phi} = a\phi + b\phi^3 - \kappa\nabla^2\phi. \tag{5}$$

An inhomogeneity in the chemical potential of local amplitude $\boldsymbol{\nabla}\mu$ will give rise to a diffusive flux, leading to the growth or depletion of the volume phases [**?**]. To model the diffusive flux, we use the constitutive equation

$$\mathbf{j} = -M\boldsymbol{\nabla}\mu, \tag{6}$$

where M, called the mobility, plays the role of a diffusion constant. Imposing local conservation of the phase field ϕ leads to the convection-diffusion equation

$$\frac{\partial\phi}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}\phi = M\nabla^2\mu. \tag{7}$$

Apart from diffusive transport of the phase field, inhomogeneities in the chemical potential give rise to a force per unit volume $-\phi\boldsymbol{\nabla}\mu$ acting on the fluid [**?**]. This term amounts to capillary stresses originating from distortions of the interface, and gives rise to the Laplace pressure of a curved interface in the sharp-interface limit. Therefore, the mass and momentum balance equations are

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = 0, \tag{8}$$

and

$$\frac{\partial(\rho\mathbf{v})}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\rho\mathbf{v} = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot(\eta(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\mathbf{v}^\mathrm{T})) - \phi\boldsymbol{\nabla}\mu. \tag{9}$$

An important aspect of the diffuse-interface approach is the ability to model contact-line dynamics. In sharp-interface approximations, imposing the no-slip boundary

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condition at the contact line leads to a diverging viscous stress [**?**], commonly known as the Huh-Scriven paradox [**?**]. In the phase-field model, this is regularized by virtue of mass diffusion, which leads to a contact-line slip velocity profile over a characteristic length scale $l_{\mathrm{D}} = \sqrt{M\eta}$ [**?**]. The emergent slip length is set by l_{D} and shows the limiting scalings $l_{\mathrm{s}} \sim \sqrt{l_{\mathrm{D}}\xi}$ [**?**] for $l_{\mathrm{D}} \ll \xi$ and $l_{\mathrm{s}} \sim l_{\mathrm{D}}$ [**? ?**] for $l_{\mathrm{D}} \gg \xi$ with a cross over between the two regimes occurring at $l_{\mathrm{D}}/\xi \approx 0.4$ [**?**].

In order to integrate the phase-field model numerically we use a Lattice-Boltzmann (LB) algorithm. Here we summarize the simulation setup and focus on the simulation results. We refer the reader to Ref. [**?**] for details of the numerical algorithm. We consider a rectangular simulation domain of dimensions $L_x \times L_y \times L_z$, discretised into N lattice sites. The size of the simulation domain was fixed using $L_x = 120$, $L_y = 100$ and $L_z = 40$. The cantilever dimensions, $l \times w$ were set to $l = 100$ and $w = 24$, and the minimum gap thickness to $h = 10$. In simulation units, the density and viscosity of the fluid are set to $\rho = 1$ and $\eta = 10^{-1}$ throughout the lattice. The bulk free-energy parameters are set to $-a = b = 3.05 \times 10^{-3}$ and $\kappa = 7.8 \times 10^{-3}$, giving a surface tension $\gamma = 4.6 \times 10^{-3}$ and an interface thickness $\xi = 1.13$. The initial condition of the fluid-fluid system is chosen by initializing the phase field to local equilibrium values, $\phi = -1$ for a gas site and $\phi = +1$ for a liquid site.

Hard walls in the lattice Boltzmann algorithm are implemented by means of the standard bounce back rules, which recover the impenetrability and no-slip boundary conditions. The interaction with the solid boundaries is prescribed by locally fixing the surface energy parameter, κ_{s}, and enforcing the boundary condition (3). For hydrophilic levers, we use $\kappa_{\mathrm{S}} = -2.8 \times 10^{-3}$, leading to $\theta_{\mathrm{e}} \approx 30°$. To model hydrophobic levers we use $\kappa_{\mathrm{S}} = 2.8 \times 10^{-3}$, which gives $\theta_{\mathrm{e}} \approx 150°$.

To drive a phase change, we follow the algorithm presented in Ref. [**?**] and fix the value of the phase field at the left end of the simulation box to a prescribed value ϕ_0. From (5) the local chemical potential is $\mu_0 \simeq a\phi_0 + b\phi_0^3$, while $\mu \approx 0$ at the interface, leading to a phase-change rate $E_0 = |\mathbf{j}|/\Delta\phi \simeq M\mu_0/\Delta\phi l_0$, where $\Delta\phi = 2$ is the difference between the bulk values of the phase field and l_0 is the average distance from the interface to the simulation box edge. We use $\phi_0 = -1.2$, which ensures that the timescale of mass diffusion is fast compared to the evaporation timescale of the front.