Extended Large-Q Potts Model Simulation of Foam Drainage

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We study the vertical liquid profile of foam drainage using the three-dimensional large-Q Potts model extended to include gravity. Forced drainage with constant rate liquid input from the top of the foam produces a constant profile. In free drainage, without liquid input from the top, homogeneously distributed liquid drains to the bottom of the foam until capillary effects and gravity balance. For pulsed drainage, as liquid drains from the top of the foam into the dry foam, a sharp interface between the wet and dry foam develops. The fixed profile moves downward at a constant velocity with a flat interface. The results of our simulations are suggested in both experiments and simplified mean-field analytical results.

Foams are of practical importance in applications as diverse as brewing, lubrication, oil recovery, and fire-fighting. Characterizing their structure and evolution present challenges to current theory and experiments. Best understood is coarsening resulting from diffusion of gas between cells. The explanation of anomalies in coarsening data has focused on the role of Plateau borders, the liquid-filled regions at the intersection of cell walls, often ignored in the study of foams with a small liquid fraction. In the case of three-dimensional liquid foams, an additional complication is the vertical drainage of the liquid due to gravity, until gravity and capillary effects balance. Often drainage, rather than diffusion, determines foam stability and properties. Many applications require detailed understanding of drainage. Mysels, Shinoda and Frankel (1959) were the first to investigate the different types of thin-film drainage, concentrating on vertical films formed by withdrawal of glass frames from pools of surfactant solution. Princen (1986) has discussed the asymptotic vertical equilibrium profile of drainage by considering the osmotic pressure of foams. Gol'dfarb, Kann and Sreiber (1988) studied the microflow in Plateau channels in relatively dry foams, and proposed a soliton solution under a mean-field assumption for liquid flow in foam. Because the foam is inhomogeneous and resembles a porous medium, we might expect that the penetration of water into the foam would result in an unstable interface or in viscous fingering. Instead, the mean-field theory predicts a flat interface.

Experiments, measuring the drained liquid as a function of time, do not offer much immediate insight (Bikerman 1953). Recently Weaire, Pittet, Hutzler and Pardal (1993) and Hutzler, Verbist, Weaire and van der Steen (1995), introducing liquid from the top of the foam, measured the velocity of the interface between the dry and wet foams in terms of the flow rate. Their AC capacitance measurement provided information on the vertical liquid profiles for different types of drainage, but could not distinguish horizontal wetness changes.

Magnetic resonance imaging (MRI) offers a non-invasive method for measuring the interior structure of foams. One-dimensional vertical wetness profiles of draining beer foams, whipped cream, and egg white, etc. have been measured by German and McCarthy (1989) and by Heil, McCarthy, German and McCarthy (1990). Gonatas, Leigh, Yodh, Glazier and Prause (1995) have successfully imaged two-dimensional sections and obtained area distributions. Prause, Glazier, Gravina and Montemagno (1995) have taken images of three-dimensional foams with very high resolution, yet full three-dimensional drainage experiments remain to be done.

The large-Q Potts model simulates the coarsening of foams (Glazier, Anderson and Grest 1990), especially in one-phase systems, and can be easily extended to include drainage. In the model, the pattern is subdivided into a regular three-dimensional lattice, with each cell assigned a unique 'spin' identification, σ, ranging from 1 to Q ($Q > 10000$ in our simulations). A cell, σ, is the collection of lattice sites $\mathbf{i} = (x, y, z)$ with spin $\sigma(\mathbf{i}) = \sigma$. We work with a two phase system, where the liquid is represented as a cell of special type. Including the gravitational field, the extended Potts Hamiltonian of the system is then:

$$\mathcal{H}_{Potts} = \sum_{\mathbf{i},\mathbf{i}' neighbours} J_{\sigma,\sigma'}[1 - \delta_{\sigma(\mathbf{i}),\sigma(\mathbf{i}')}] + \sum_{liquid} g\ y_{liquid}, \tag{1}$$

where $J_{\sigma,\sigma'}$ is the coupling constant between different types, in this work, $J_{gas,gas} > J_{gas,liquid} > J_{liquid,liquid}$; δ is the Kronecker delta function; g is the force of gravity per unit density and y_{liquid} is the height of the liquid component of the foam. The second term in $\mathcal{H}_{Potts}$ applies to the liquid only. At each time step, a site and trial spin are selected at random. Substitutions are made with probability P,

$$P = \begin{cases} 1 & \Delta H < 0 \\ 0.5 & \Delta H = 0 \\ exp(-\Delta H/T) & \Delta H > 0 \end{cases}$$

where ΔH is the change in $\mathcal{H}_{Potts}$ due to flipping a trial spin. One Monte Carlo step (MCS) consists of as many trials as there are lattice sites.

To reduce lattice anisotropy effects, we use fourth-nearest-neighbor-interaction, which is known to evolve in a manner very close to ideal isotropic grain growth (Holm, Glazier, Srolovitz and Grest 1991).

In our simulations, applying a periodic boundary condition for liquid in the y direction (the direction of gravity), corresponds to adding liquid at the top of the foam at a constant rate, called forced drainage. Free drainage has no input of liquid over time and the liquid has a homogeneous initial distribution in the y direction. In pulsed drainage, the foam is initially dry and a fixed amount of liquid initially placed above the dry foam drains under gravity. Note that we start our simulations from a very ordered initial condition of stacked parallelepipeds, which affects the shape of the interface between the wet and dry foam in pulsed drainage. We study draining processes by monitoring the liquid profiles of drainage, i.e., the liquid fractions as a function of height.

Theoretical calculations of the liquid flow during foam drainage assume that the liquid flows through a system of interconnected, randomly oriented Plateau channels, with negligible flow through the soap films. When the gravitational force predominates over the capillary forces, as is usually true in foams, the outflow process may be regarded as a kinematic wave described by Burger's equation (Gol'dfarb *et al.* 1988; Verbist and Weaire 1994). Since we do not consider the details of foam properties such as bubble size distribution, bubble density and liquid viscosity etc., this is indeed a mean-field approximation.

In analysing liquid motion along the channels and films in foam, difficulties arise in determining the conditions at the interphase boundaries. In order to make a stable foam, surfactants are usually added to the liquid. A monomolecular layer of surfactant on the surface interacts with the liquid molecules, which not only reduces the surface tension but also stabilizes the surface layers of the liquid, retarding the liquid motion. Thus we assume, as a first approximation, non-slip conditions on the boundaries.

The capillary pressure, i.e. the pressure across the liquid surface, is

$$P_l - P_g = \frac{2\gamma\cos\theta}{r}, \tag{2}$$

where γ is the surface tension, θ is the contact angle between liquid and gas, r is the radius of curvature of the lateral surface of the Plateau border, and p_l and P_g are the pressure of liquid and gas, respectively. Since δP_l is usually negligibly small compared to P_g, we have the relation between the change of gas pressure δP and the change in the channel area δs:

$$\delta P = \gamma\alpha s^{-3/2}\delta s, \tag{3}$$

where α is a constant determined by r. For ideal Plateau borders, $\theta = \pi/3$, and r can be related to the area of the Plateau border s by $s = (\sqrt{3} - \pi/2)r^2$, yielding $\alpha = (\sqrt{3} - \pi/2)^{\frac{1}{2}}$ in this special case.

If we treat the internal hydrodynamics of foams on the basis of the continuum mechanics of multiphase media, namely, we assume the motion of the liquid in the Plateau channels to be microscale flow and ignore the detailed structure of foams, we can apply the continuity equation to the channel flow:

$$\frac{\partial s}{\partial t} + u\frac{\partial s}{\partial x} + x\frac{\partial u}{\partial x} = 0, \tag{4}$$

with u being the velocity of the flow, and the liquid being treated as incompressible.

The ratio of the pressures due to gravity and capillarity is

$$\begin{aligned} P_{gravity} : P_{capillary} &= \rho g h : \frac{2\gamma\cos\theta}{r} \\ &\sim \frac{\rho g h r}{2\gamma}, \end{aligned} \tag{5}$$

in which $\rho \sim 10^3$ kg$/m^3$, $g \sim 10$ kg m $/s^2$. For a moderately wet foam ($\sim 10\%$ of liquid) both h, the height of the liquid channels, and r, the radius of curvature of the lateral surface of plateau borders, are of the same order of magnitude as the size of a single cell. Thus $h \sim r \sim 10^{-2}$ m. The surface tension γ is lower than that of water 10^{-2} N/m. By a crude order of magnitude argument, we show $P_{gravity}$ is at least two orders of magnitude larger than $P_{capillary}$. Hence capillary effects are negligible compared to gravity in wet foams. Only in the dry form limit or in the late stages of drainage, when r can be as small as the film thickness, will the capillarity contribution to the driving force be significant.

Following the derivation in Gol'dfarb *et al.* (1988), we consider the solution of the Navier-Stokes equation for a tube of arbitrary cross-section in the case of ponderable fluid:

$$u = -\frac{s}{\beta\eta}\left[\frac{1}{3}\frac{\partial P}{\partial x} - \rho g\right], \tag{6}$$

where η is the dynamic viscosity of the fluid; the factor 1/3 comes from averaging over the directions of motion of the liquid, and β is a numerical coefficient depending only on the shape of the cross-section of the channel, e.g. $\beta = 8\pi$ for a tube of circular section, $\beta = 49.1$ is obtained for a cross-section in the form of a Plateau triangle by carrying out a numerical integration of the Navier-Stokes equation. Combining (4) and (6) yields the evolution equation of sectional area of plateau border

$$\frac{\partial s}{\partial t} + s\frac{\partial s}{\partial x} = \beta\frac{\partial}{\partial x}(s^{1/2}\frac{\partial s}{\partial x}), \tag{7}$$

where all the variables are reduced, i.e., dimensionless. The steady profile solution to (7) is

$$s = 2v \tanh^2[\frac{\sqrt{v}}{\beta}(x - vt)] \tag{8}$$

The solution to the channel area is a hyperbolic tangent function, namely, a solitary wave that moves at a constant velocity.

In figure 1, we plot the liquid profile for simulated forced drainage. Unlike in the experiments of Hutzler *et al.* (1995), the forced drainage studied here has an initial condition with liquid homogeneously distributed in the vertical direction. The profiles stay the same over time within their fluctuation amplitude, indicating the equilibrium between the constant liquid input from the top of the foam and gravity.

Figure 2a shows the time evolution of the liquid profiles in free drainage. With no liquid input, the initially homogeneously distributed liquid drains downwards until gravity balances capillary effects, when an equilibrium profile is reached. Drainage profiles from MRI experiments by German *et al.* (1989) and Heil *et al.* (1990) and our group(figure 2b) are very similar, though it is hard to compare them quantitatively. Effort has been made to quantify the slope of the linear part of the profile without much success.

For pulsed drainage, a fixed amount of liquid is put on top of the dry foam at time zero. The pulse is monitored as it moves downward. The time evolution of the liquid profiles is shown in figure 3. The high-frequency structure of the pulses is due to the ordered structure of the simulated foams, as can be seen from figure 4, showing snapshots of the vertical cross-section of pulsed drainage. The leading edge of the pulse, despite the fact that it decays slightly in height over time, is quantitatively identical to the soliton in the experiments of Hutzler *et al.* (1995). In fact, in figure 3, we fit the leading edges of profiles at 4000 MCS and 6000 MCS with the same soliton solution (equation 8). A longer time simulation (long travelling distance for the pulse in the y direction) should be able to see liquid transfer from the peak of the soliton to the tail, resulting in the pulse spreading out. Thus over the timescales we investigate, the leading edge of the pulse behaves indistinguishably from a soliton. We are currently simulating true solitons in disordered froths. The ordered structure of the foam is a much larger perturbation. The wave front position of the pulse is plotted against time in figure 5, showing a constant velocity. We also observe that when the coarsening of the foam is comparable to draining, the interface between the wet and dry foam is not sharp due to the disordered structure. The liquid forms clusters in the middle of the foam resembling viscous fingering. Only when the draining process is much faster than coarsening can we see a sharp interface. In this case the interface is indeed flat, ranging within a very narrow vertical band (smaller than the dimension of a bubble), which has not been observed before. We are currently studying pulsed drainage starting from an initally coarsened foam to see how the configuration affects the shape of the interface between the wet and dry foam.

Thus the extended large-Q Potts model simulations, assuming only the energy minimization, produce results comparable to experiments and also validate the mean-field drainage theory. Modification of the extended Potts model should allow the quantitative comparison of liquid profiles with experiments, study of the effects of foam density, liquid viscosity and surface tension on the foam drainage, and quantitative simulations of the properties of industrial foams.

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FIGURE CAPTIONS

Figure 1. Liquid profiles for forced drainage (constant for all time).

Figure 2. Liquid profiles for free drainage as a function of time: (a) Potts model simulation. (b) MRI experiment data.

Figure 3. Liquid profiles for pulsed drainage as a function of time. Simulation time is in terms of Monte Carlo steps (MCS). Leading edges of pulses at 4000MCS and 6000MCS are fitted with soliton solution (* lines).

Figure 4. Snapshots of vertical cross-section of pulsed drainage: (a) 0 MCS. (b) 8000 MCS. (c) 11000 MCS.

Figure 5. The wavefront propagation of the soliton for pulsed drainage.