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Rheological properties of the soft-disk model of two-dimensional foams

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The soft-disk model previously developed and applied by Durian [D. J. Durian, *Phys. Rev. Lett.* **75**, 4780 (1995)] is brought to bear on problems of foam rheology of longstanding and current interest, using two-dimensional systems. The questions at issue include the origin of the Herschel-Bulkley relation, normal stress effects (dilatancy), and localization in the presence of wall drag. We show that even a model that incorporates only linear viscous effects at the local level gives rise to nonlinear (power-law) dependence of the limit stress on strain rate. With wall drag, shear localization is found. Its nonexponential form and the variation of localization length with boundary velocity are well described by a continuum model in the spirit of Janiaud *et al.* [*Phys. Rev. Lett.* **97**, 038302 (2006)]. Other results satisfactorily link localization to model parameters, and hence tie together continuum and local descriptions.

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I. INTRODUCTION

A. Foam rheology

While the deformation and flow properties of foams are broadly understood in terms of shear elastic modulus, yield stress, etc. [1–3], many details remain perplexing. A fuller understanding must address both the local forces that operate at the level of the individual films, and the way in which these forces combine to determine the overall response to strain. This paper will be entirely devoted to the second question. It uses a particularly simple representation of bubbles and their mutual forces, as previously developed by Durian [4–7]. This model may be unrealistic in some respects, but its simplicity and computational tractability makes it attractive at a time when more precise descriptions of dynamic properties are lacking.

Our immediate goal is to thoroughly analyze the properties of this model, *per se*. Since it represents bubbles as soft disks [in the two-dimensional (2D) case] it has some relevance to granular materials as well. As is often the case in foam physics, this study will remain for the time being in two dimensions, which has obvious advantages. The main experimental literature of foam rheology is concerned with ordinary three-dimensional (3D) foams, but in recent years, considerable attention has been focused on their 2D counterparts.

It has turned out that the obvious 2D experimental sample, consisting of foam trapped between two plates [see Fig. 1(c)], has shear properties that are significantly affected by viscous drag forces exerted by the confining plates. We will therefore be concerned with two quite different but related cases: with and without such forces. The latter case can be realized experimentally in 2D as a Bragg raft [Fig. 1(a)] and it is roughly analogous to a 3D foam, because of the

absence of confinement-induced forces. Having defined the model, we will deal with this case first, and proceed to introduce the wall forces at a later stage. In summary, the main goals of this work are (1) to extract the parameters of a continuum (Herschel-Bulkley) formalism, by means of simulation, and (2) to use these in a continuum model for 2D shear localization. Both of these goals are satisfactorily realized within the scope of the present calculations.

B. Questions raised by experiments

It is necessary first to review some of the history of foam rheology. The more traditional 3D experiments, for example, those of Khan *et al.* [8], have used various types of rheometers to explore the relation between stress, strain, and strain rate. This is most straightforward when strain rate does not change sign; that is, increments of shear are always in the same sense, and we shall adopt that restriction here also. Awkward complications arise from hysteretic effects in the more general case [9]. The conclusion has generally been that the data is well accounted for by the Herschel-Bulkley equation. This adds to the quasistatic stress-strain relation a second term proportional to the strain rate $\dot{\gamma}$, raised to the power a ,

$$\sigma = \sigma_y + c_v \dot{\gamma}^a, \quad (1)$$

where σ and σ_y denote, respectively, stress and yield stress, c_v is the viscosity component of stress (also called *consistency*), and a is the Herschel-Bulkley exponent. However, the exact value of a is still subject to debate. Most experiments agree on the shear-thinning behavior of foams, whereas for $a=1$ (the Bingham fluid), the effective viscosity (that is, stress divided by strain rate), tends to *constant* at high rate of strain, it tends to *zero* if $a < 1$. While Schwartz and Princen [10] predicted theoretically that $a=2/3$, various values between 0.25 and 1 have been measured experimentally (see, for instance, [8,11–16]). Besides, Denkov *et al.*

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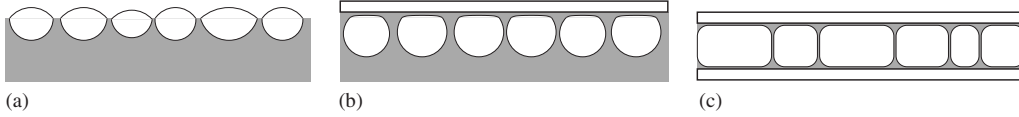


FIG. 1. Three types of 2D foams: (a) monolayer of air bubbles sitting at liquid/air interface (Bragg raft); (b) bubbles floating in liquid under a glass plate; and (c) bubbles confined between two glass plates. There are large effects due to the drag associated with motion relative to solid boundaries in both (b) and (c).

[14] and Katgert *et al.* [15] showed, respectively, that a depends on the properties of the surfactant and on the polydispersity of the foam. The obvious question arises: what determines the value of a ? There has been little understanding of this up until now, and it is one of our stated objectives to explore the question within the context of a simple model.

A second question concerns normal stresses or the related phenomenon of dilatancy. While often mentioned in the context of granular materials, these effects have not been much considered for foams, apart from the work of Weaire and Hutzler [17,18], confined to the quasistatic case. As they noted, there is, in principle, a second and possibly more important *dynamic* contribution to these effects, well known to rheologists [19,20]. So one may ask: what are the dynamic effects in a simple model?

As in much of foam physics, recourse may be made to two-dimensional systems, for the sake of simplicity and transparency. We will not attempt a full review of the various rheological experiments on 2D foams that have been performed over the last five years [13,15,21,22]. Equally, we will give no details of the quasistatic calculations [23,24] that have been adduced to account for them, or the continuum theory [25–28] which has offered an alternative viewpoint. We will argue that the present paper strongly supports the continuum model. Some results of the quasistatic calculations suggest that corrections are needed to account for the role of polydispersity, and we do not rule that out.

C. Soft sphere or disk model

In the model developed by Durian around 1995, 2D bubbles are represented by circular disks. When overlapping (and only then) they interact via a simple spring force, the displacement of the spring being the radial overlap (see Fig. 2). The elastic repulsive force \mathbf{F}_n acting on bubble i due to bubble j is given by

$$\mathbf{F}_n = \kappa \frac{2R_0}{R_i + R_j} \Delta_{ij} \mathbf{n}_{ij}. \quad (2)$$

Here κ is the coefficient of elasticity, \mathbf{n}_{ij} is the normal vector between bubbles i and j ,

$$\mathbf{n}_{ij} = \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (3)$$

and the overlap Δ_{ij} (see Fig. 2) is given by

$$\Delta_{ij} = \begin{cases} (R_i + R_j) - |\mathbf{r}_i - \mathbf{r}_j| & \text{if } (R_i + R_j) < |\mathbf{r}_i - \mathbf{r}_j| \\ 0 & \text{otherwise.} \end{cases} \quad (4)$$

R_i and R_j are the radii of bubbles i and j , centered at \mathbf{r}_i and \mathbf{r}_j , respectively, and R_0 is the average bubble radius of the

entire bubble packing. The ratio $\frac{2R_0}{R_i + R_j}$ in Eq. (2) takes into account that larger bubbles are easier to deform than smaller ones. In such a model one may define an effective liquid fraction ϕ (which ignores the overlap of disks) as $\phi = 1 - N\langle R_0^2 \pi \rangle / A$, where A is the area of the confinement of the disks and N is the total number of disks. Since a packing of polydisperse disks loses its mechanical rigidity for $\phi > 0.16$, for higher values of ϕ it no longer represents a two-dimensional foam. In all the following, the liquid fraction will be chosen as $\phi = 0.05$.

A real flowing foam dissipates energy by viscous friction in the films and Plateau borders separating the bubbles. The films are not explicitly represented in our model. The simplest expression, as used by Durian [5] and adopted here, represents the viscous force \mathbf{F}_d on bubble i associated with a neighboring bubble j as

$$\mathbf{F}_d = -c_b (\mathbf{v}_i - \mathbf{v}_j), \quad (5)$$

where c_b is the dissipation constant for the bubble-bubble interaction and \mathbf{v}_i and \mathbf{v}_j are the respective bubble velocities. With all the above definitions, the model can provide a semi-quantitative description of foams throughout the range of liquid fraction consistent with stability. In Durian's original calculations [5], inertia was neglected. Hence all forces on each bubble were balanced. This reduces the problem to a set of linear equations in the velocities of the bubbles. Durian then further simplified the problem by substituting the viscous drag exerted on each bubble by its neighbors to the value the drag would have in a linear velocity profile. He thus sets the average velocity $\langle \mathbf{v}_j \rangle$ of all neighbors j of bubble i to $\langle \mathbf{v}_j \rangle = \dot{\gamma} y_i \hat{\mathbf{x}}$, where $\dot{\gamma}$ is the imposed strain rate and y_i is the y coordinate of bubble i .

In our calculations we instead allow each bubble to move independently, subject to the elastic and dissipative forces

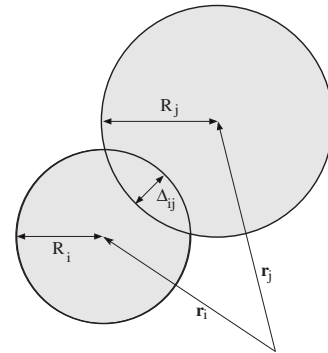


FIG. 2. Overlap Δ_{ij} between two contacting bubbles of radii R_i and R_j , located at \mathbf{r}_i and \mathbf{r}_j , respectively.

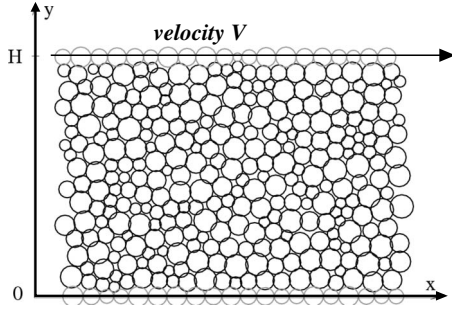


FIG. 3. Snapshot of 2D soft-disk foam. The sample is periodic in the horizontal direction; bubbles at the upper and lower boundary are shown in gray. In the simulation the upper boundary is moved with velocity V .

defined above. In practice we used the Verlet algorithm, with a bubble mass m_b small enough to assume that inertial effects are negligible (the ratio $\kappa m_b / c_b^2$ was set to 0.01). We present results here only for the eventual steady state after long times. The results obtained are significantly different from those of Durian. This may be due to the strong approximation that he used, as indicated above. This approximation had been removed later by Tewari *et al.* [6], but they were not interested in the rheological properties and concluded that both versions of the model were equivalent.

II. RESPONSE TO SIMPLE SHEAR IN THE ABSENCE OF WALL DRAG

A. Herschel-Bulkley power-law exponent

In this section we deal with the Durian model, with no additional viscous drag force from confining plates. Our first computations concerned the evaluation of its flow properties under simple shear, in particular, the value of the Herschel-Bulkley power-law exponent a in Eq. (1). To this purpose we generated assemblies of 1000–10 000 bubbles in a rectangular confinement, as shown in Fig. 3, using periodic boundary conditions in the horizontal direction. The bubbles at the upper boundary, which are treated as attached to this boundary, are given a constant velocity V . This corresponds to the application of strain at a constant rate $\dot{\gamma} = V/H$ for a sample of width H (see Fig. 3). We will only consider polydisperse foams, the bubble radii having a uniform distribution within the range $R = R_0(1 \pm 0.15)$.

At this stage it is convenient to introduce a dimensionless Deborah number De , which is defined as the ratio of the characteristic time of the material that is sheared to the characteristic time of the deformation process [29]. We identify the latter with $\dot{\gamma}^{-1}$, and the material time scale we relate to the competition of energy storage and dissipation at the level of bubble-bubble interactions. This then results in the definition $De = \dot{\gamma} c_b / \kappa$.

Under an imposed boundary shear, after a transient, the system of disks reaches a steady average state. It is characterized by a linear average velocity profile of the disks with regard to their vertical position in the sample, so there is no localization in the present case; we may proceed to extract the constitutive law in a straightforward way. We determine

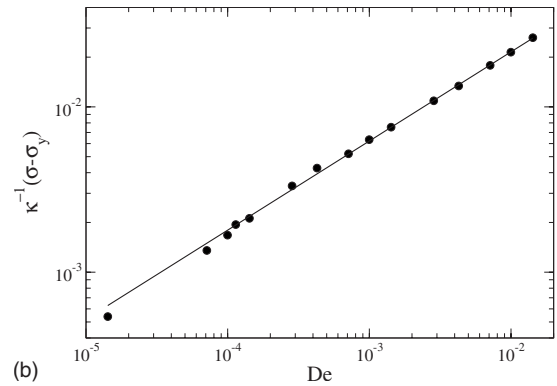
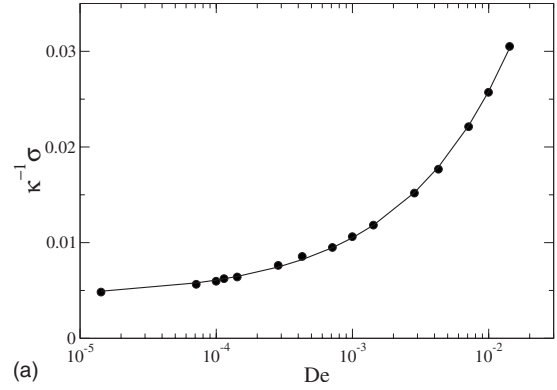


FIG. 4. (a) Stress on the moving boundary as a function of the Deborah number $De = \dot{\gamma} c_b / \kappa$. The solid line is a fit to Eq. (1) (reexpressed in terms of De), resulting in the Herschel-Bulkley exponent $a = 0.54 \pm 0.01$. In (b) we have subtracted the fitted value of the yield stress σ_y from the data to show the power-law behavior in a double logarithmic plot.

the stress at the moving boundary as a function of V . In Fig. 4 we display this variation as a function of the dimensionless Deborah number De . A least-square fit of the data with the Herschel-Bulkley form results in

$$\sigma / \kappa = 0.0043 + 0.26 De^{(0.54 \pm 0.01)}. \tag{6}$$

The model foam thus exhibits a strongly nonlinear, shear-thinning rheological behavior, despite the linearity of all local forces. This can be attributed to the importance of disorder in such a polydisperse jammed system: the velocity fluctuations cannot be neglected and make the trajectories of the bubbles strongly nonaffine. Therefore the simple image of bubble layers sliding over each other is misleading. In the initial version of the model applied by Durian [4,5], the mean-field approximation effectively subtracts these disordered motions, which results in a Bingham rheology ($a = 1$). Let us note that the nonlinear behavior does not affect the average velocity profile in the simple shear geometry we adopted (as opposed to what happens in a cylindrical Couette geometry [13]). The shear localization that is discussed in later sections is not seen here.

The value of the Herschel-Bulkley exponent we obtain [Eq. (1)] $a = 0.54 \pm 0.01$ is roughly consistent with the various experimental measurements already mentioned, that showed a nonlinear, shear-thinning behavior [8,11–16].

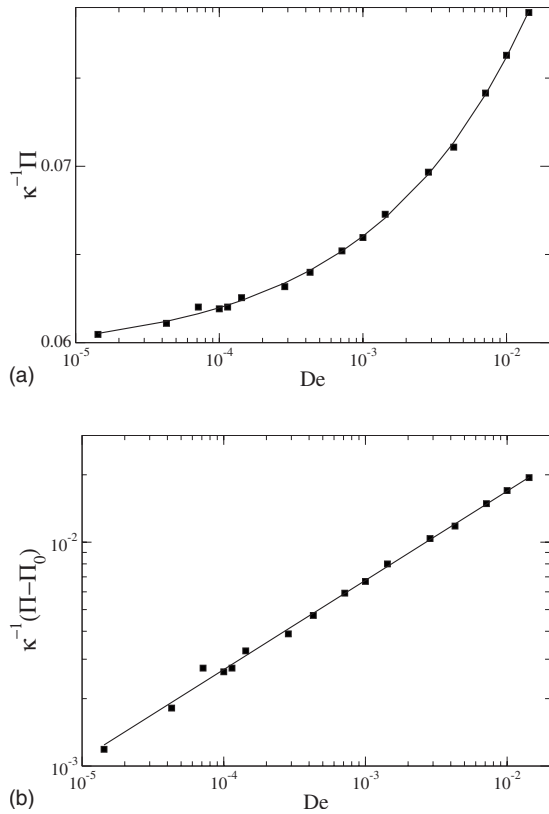


FIG. 5. Pressure acting on the moving boundary as a function of the Deborah number. The data is well described by Eq. (7) with an exponent 0.4 ± 0.01 . In (b) we have subtracted the fit parameter Π_0 to show the power law behavior in a double-logarithmic plot.

However, it is slightly higher than most experimental values. This discrepancy can be attributed to the extreme simplicity of the local ingredients of the model that we have used here. Including more realistic forces at the local scale might lead to a better estimation of the Herschel-Bulkley index. Recent theoretical work by Denkov *et al.* [30] implies that the viscous dissipation between two bubbles sliding along each other should scale like $\Delta V^{1/2}$ rather than being linear. However, the relation between the local properties and the macroscopic rheology is still not understood. Further work on this topic is currently performed and will be the subject of a subsequent publication.

B. Normal stress

In a system constrained by a fixed applied pressure, the foam would expand in volume (by increasing its nominal liquid fraction) when sheared. In our simulations we impose the volume by fixing the position of the edge bubbles, and measure the resulting pressure Π on the boundaries. Its variation with shear rate is shown in Fig. 5 and is well described by a formula analogous to the Herschel-Bulkley equation,

$$\Pi/\kappa = 0.059 + 0.11De^{(0.40 \pm 0.01)}. \quad (7)$$

For the case of $De=0$ one obtains the static osmotic pressure of the foam, Π_0 [17]. Although the tendency of a 3D foam to

increase its liquid fraction under shear has been qualitatively reported in experiments [31], we do not know of any quantitative experimental measurements of the dynamic variation of the osmotic pressure, which is particularly difficult to obtain in 2D. Rheologists sometimes cite the old work of Baginold [19] as indicating a *quadratic* dependence, very different from the power law in Eq. (7). We have not proceeded any further with the analysis of the normal stress.

III. EFFECT OF WALL DRAG

A. Adding wall drag

As we have already mentioned, certain experiments with a 2D foam between two glass plates exhibit a new type of flow; when one boundary is moved to produce shear, the resulting shear is exponentially localized at that boundary [22]. According to the continuum model of Janiaud *et al.* [25–27] this is to be understood as a direct effect of the wall drag, which we will now introduce into the numerical model. This continuum model in its original form assumed a constitutive equation of the Bingham type ($a=1$), and added in the drag force F_w , as a body force proportional to local velocity. This predicted an exponential localization of the flow along the moving boundary, the width of the shear band being independent of the driving velocity.

To mimic that theoretical model in our simulations, we now add to the forces acting on bubble i , a wall drag force \mathbf{F}_w , given in the most simple form by

$$\mathbf{F}_w = -c_w |\mathbf{v}_i|^b \frac{\mathbf{v}_i}{|\mathbf{v}_i|}, \quad (8)$$

where c_w is a drag constant. According to Bretherton [32] and Denkov *et al.* [14], for surfactants with low surface viscosities, the friction of the foam due to the wall is characterized by $b=2/3$. However, to keep all the ingredients of our model linear, we will adopt $b=1$. The resulting equation of motion is again solved numerically, using the second order Verlet method. Note that we have just established in Sec. II A that the appropriate constitutive law is not that of Bingham, so we will have cause to return to this point again. As we shall see, the results for the steady shear at long times exhibit localization, which conforms well to the prediction of the continuum model.

B. Flow localization

Shear simulations with added wall drag were performed on an assembly of 10 000 soft disks, for constant values of $\chi=c_b/c_w$, the ratio of dissipation and drag constant. Once a steady state was reached, we determined the velocity profile between static and moving boundary by performing time averages over the horizontal velocity components of the bubbles. While in the absence of wall friction ($c_w=0$, i.e., $\chi \rightarrow \infty$), the velocity profile is roughly linear throughout the sample, this is no longer the case for finite values of χ . Instead, flow is localized near the moving boundary, as shown in Fig. 6. A localization length $\lambda_{1/10}$ can be arbitrarily defined by measuring the distance from the moving boundary at which the velocity reaches 1/10th of its value at the

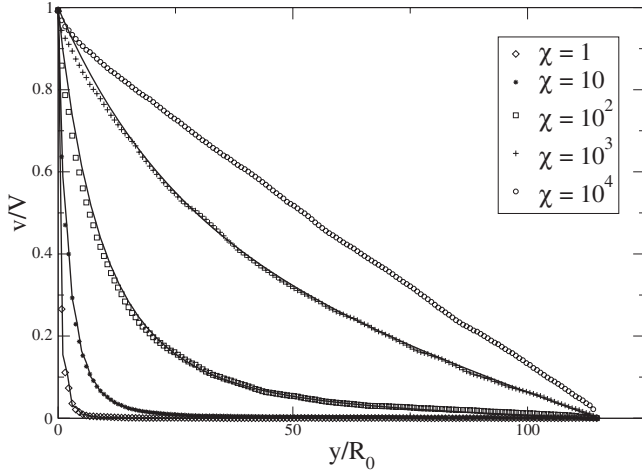


FIG. 6. Normalized velocity profiles in the foam for a range of values of the parameter $\chi = c_b/c_w$. Shear close to the moving boundary is enhanced as wall friction is increased, i.e., with decreasing χ . The solid lines, which agree closely with the data, were obtained numerically from the continuum model, using the Herschel-Bulkley index $a=0.54$.

boundary (see also the Appendix). The variation of $\lambda_{1/10}$ with χ is shown in Fig. 7. For values of $\chi \leq 500$ (i.e., if the shear band width is less than the sample width H) the localization length varies with χ in the form of a power law, $\lambda_{1/10} \propto \chi^{0.64 \pm 0.01}$.

Figure 8 shows the evolution of $\lambda_{1/10}$ with the Deborah number De , when varying the driving velocity V . A least-square fit results in

$$\lambda_{1/10}/R_0 = 0.87De^{-0.30}. \quad (9)$$

Such a power-law scaling can also be found theoretically by modifying the continuum model of Janiaud *et al.* [25] to incorporate the Herschel-Bulkley rheology we exhibited here: the velocity field $v(y)$ has to be such that the internal

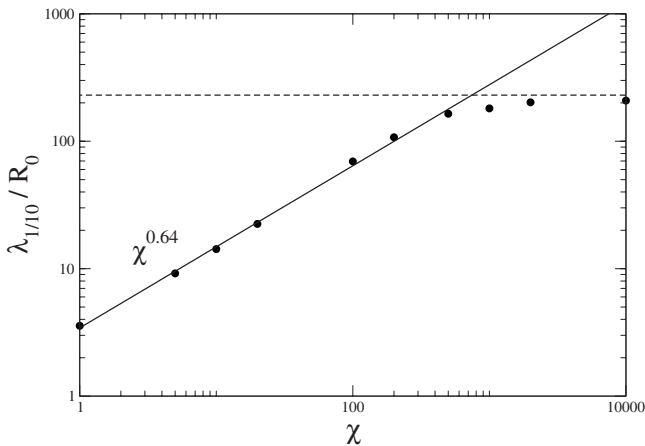


FIG. 7. Localization length $\lambda_{1/10}$ as a function of the dimensionless ratio $\chi = c_b/c_w$. The solid line is a fit of the data for $\chi < 500$ to a power law, resulting in $\lambda_{1/10}/R_0 \propto \chi^{0.64 \pm 0.01}$. The power-law behavior is limited by the width of the sample, which is indicated by the dashed line (in units of the average bubble radius R_0).

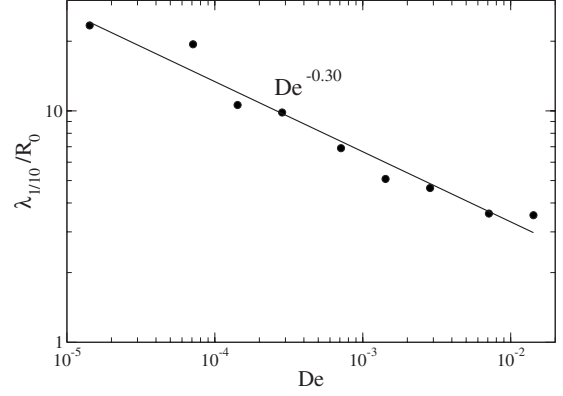


FIG. 8. Normalized localization length $\lambda_{1/10}/R_0$ as a function of the Deborah number. The solid line is a fit of the data to a power law, resulting in $\lambda_{1/10}/R_0 = 0.87De^{-0.30}$, in excellent agreement with theory. (Here the sample width was $28R_0$.)

dissipation is exactly balanced by the friction along the confining plates; that is,

$$c_v \frac{d}{dy} \left[\left(\frac{dv}{dy} \right)^a \right] = c_d v(y)^b. \quad (10)$$

Here c_d is the wall drag constant c_w of Eq. (8) per unit area, i.e., $c_d = c_w / (\pi R_0^2)$ and $b=1$ for the case of the simple linear form for the drag force considered here. The exponent a is the one from the Herschel-Bulkley relationship, i.e., $a = 0.54$ in our case [see Eq. (6)], and c_v is the viscosity component of stress. This equation can be solved to predict the localization of the flow, as shown theoretically in [28]: the (exponentially defined) localization length l is given by

$$l \approx \left(\frac{c_v}{c_d} \right)^{1/1+a} v^{a-b/1+a}, \quad (11)$$

provided that l is much less than the sample size (the two definitions of the localization length are related by $\lambda_{1/10} = \ln(10)l$; see the Appendix). This immediately gives the scaling $\lambda_{1/10} \propto c_w^{0.65}$, in excellent agreement with the data shown in Fig. 7. However, the success of the continuum model is not confined to such scaling relationships, but is fully quantitative. Rewriting Eq. (11) in terms of the Deborah number gives

$$l \approx \left(\frac{c_v}{c_d} \right)^{1/1+a} \left(\frac{H\kappa}{c_b} \right)^{a-b/1+a} De^{a-b/1+a}. \quad (12)$$

Inserting our simulation input parameters for c_d , H , c_b , R_0 , and $b=1$, together with our numerical results for the values of c_v and $a=0.54$, we obtain

$$l/R_0 = 0.36De^{-0.30}. \quad (13)$$

This corresponds to $\lambda_{1/10}/R_0 = 0.83De^{-0.30}$, which is also in excellent agreement with the numerical results (see Fig. 8). We have concentrated on the localization length here, but the full velocity profile, which turns out to be only approximately exponential, can be numerically calculated from it. As Fig. 6 shows, the result is in close agreement with the data.

IV. CONCLUSIONS

By means of numerical simulations based on the soft-disk model, we have shown that the Herschel-Bulkley rheology of a 2D foam can be derived from a discrete model with good agreement with experiments. Our model also predicts a dynamic dilatancy, that is, a tendency of the foam to increase its volume when sheared. Finally, we added to the classical bubble model the viscous friction experienced by a foam under confinement, which resulted in the formation of shear bands, as had been observed in experiments and derived with a continuum model. Adapting this rheological model to our parameters led to a consistent picture of the link between the local and global descriptions. This must be regarded as a strong indication for the theory, but it will be important to examine the limits of that conclusion.

Previous quasistatic simulations [24] suggest that disorder (polydispersity) plays a role. So far, our interpretation is that wall drag is responsible for localization, as prescribed by the continuum model, but that the eventual localization length contains an *additional* contribution from polydispersity, not contained within the continuum description.

In further studies, we will explore this by concentrating on the limit in which $\lambda \rightarrow 0$ for the continuum model, and seek to identify the effect of polydispersity, which is expected to be significant in that limit. It will also be informative to repeat simulations with different local forces, to try to establish the precise relation (if any) of the Herschel-Bulkley parameters to these forces. Finally, if our conclusions are sustained for this and similar models, the core theoretical problem of the origin of the Herschel-Bulkley nonlinearity will remain.

ACKNOWLEDGMENTS

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APPENDIX: DEFINITION OF LOCALIZATION LENGTH

The precise definition of localization length is, in general, arbitrary. For the analysis of our numerical results we chose to use

$$v(\lambda_{1/10}) = V/10, \quad (\text{A1})$$

where $v(y)$ is the local average bubble velocity, measured a distance y away from the boundary, which moves at velocity V .

In the continuum theory an alternative definition was used [28]

$$v(l) = V/e. \quad (\text{A2})$$

There is no general relation between these two, but since localization is, in general, approximately exponential, we may use

$$\lambda_{1/10} \approx \ln 10l \approx 2.30l \quad (\text{A3})$$

to adjust the theoretical prediction. We have adopted this procedure in Sec. III B.

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