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Free-surface dynamics of small pores

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HIGHLIGHTS

- We consider the contraction of small pores nucleated in fluid sheets.
- We characterize the pore dynamics solving the full Navier–Stokes system.
- A scaling function without free parameters describes the size of closing pores near collapse.
- Contracting pores may reverse the direction of motion (flicker) and expand.

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ABSTRACT

When the size of a pore nucleated in a fluid sheet is sufficiently small, the pore will contract and close driven by its large radial curvature. The dynamics of small contracting pores are relevant to a number of natural systems and practical applications, from fission pores in cell membranes to the fabrication of nanopores in sensors for DNA sequencing. Here, we report high-fidelity numerical simulations that provide detailed insight into the mechanisms of pore contraction and collapse in fluid sheets of low viscosity. Results uncover a scaling law that predicts the radius of a closing pore as a function of the time to collapse without free parameters. Simulations also show that contracting pores do not always proceed to collapse. Instead, some contracting pores reverse the direction of motion and expand.

1. Introduction

This paper reports a numerical study of the free-surface dynamics of small pores in fluid sheets. Unlike large pores, sufficiently small pores contract and close driven by surface tension and their large radial curvature—a behavior discussed in the pioneering work by Taylor and Michael (1973).

The dynamics of small contracting pores in fluid sheets impact a wide range of systems, from electroporation and fission pores in cell membranes to the stability of food foams (Moroz and Nelson, 1997; Wanunu, 2012; Zhao et al., 2010). Moreover, understanding and ultimately controlling the dynamics of small pores in the micro and nanoscales offer potential applications for the fabrication of sensors for rapid characterization of biomolecules and DNA sequencing (Storm et al., 2003, 2005; Dekker, 2007; Schneider and Dekker, 2012).

Although the dynamics of large expanding pores have been extensively studied and the speed of expansion is now well characterized (Culick, 1960; Taylor, 1959; Ranz, 1950; Savva and Bush, 2009; Debregeas et al., 1995, 1998; Keller et al., 1983; Keller and Mikiss, 1983), surprisingly little is known about the free-surface dynamics of small contracting pores and their speed of collapse. Indeed, in a recent theoretical and numerical work, Savva and Bush (2009) investigated the free-surface dynamics of circular pores using a lubrication model in the long wavelength limit. Their findings provided important insights into the early stage dynamics of pore expansion, and confirmed the exponential growth rate observed in experiments. However, due to limitations intrinsic to the lubrication approximation, the lubrication model cannot predict the dynamics of small contracting pores.

To study the free-surface dynamics of small pores, we have developed high-fidelity simulations that overcome the limitations of the lubrication model by solving the full Navier–Stokes (NS) equations. Here, we report how the solution of the full NS system enables a detailed analysis of the free-surface dynamics of pore contraction (Section 3.2), and uncovers a new scaling law that predicts the size of collapsing pores near the singularity without

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free parameters (Section 3.3). Results also characterize the behavior of small contracting pores that suddenly change the direction of motion and expand (flicker) by purely hydrodynamic reasons (Section 3.4).

2. Problem description

We now state our model and assumptions. We consider the free-surface dynamics of circular pores nucleated in a fluid sheet of density ρ, viscosity μ, and surface tension σ, as sketched in Fig. 1. The model and results are described in this paper using the thickness of the fluid sheet H as characteristic length scale, the inviscid time $\tau \equiv \sqrt{\rho H^3/\sigma}$ as characteristic time scale, and the stress μ/τ as characteristic pressure scale.

To analyze the pore dynamics, we numerically solved the full axisymmetric Navier–Stokes and continuity equations:

$$Re\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p+\nabla^2\mathbf{v}, \tag{1}$$

$$\nabla\cdot\mathbf{v}=0, \tag{2}$$

for the velocity $\mathbf{v}$ and pressure p. The Reynolds number $Re \equiv \sqrt{\rho\sigma H}/\mu$ based on the inviscid velocity $\sqrt{\sigma/\rho H}$ is related to the Ohnesorge number $Oh = 1/\sqrt{2}\,Re$ based on the Taylor–Culick velocity $\hat{v}_c = \sqrt{2\sigma/\rho H}$ (Taylor, 1959; Culick, 1960). We further assume that gravity can be neglected compared with surface tension. Along the sheet interface both the traction boundary condition

$$\mathbf{T}\cdot\mathbf{n} = 2\,Re\,\mathcal{H}\mathbf{n}, \tag{3}$$

and the kinematic boundary condition

$$\mathbf{n}\cdot(\mathbf{v}-\mathbf{v}_s)=0 \tag{4}$$

were imposed, where $\mathbf{T}$ is the stress tensor, $\mathbf{v}_s$ the velocity of the points at the interface, and $\mathbf{n}$ the unit normal vector to the interface (Slattery et al., 1990). The interfacial curvature is $\mathcal{H} = 1/2\,(\kappa_z+\kappa_r)$, where κ_z and κ_r are the axial and radial curvature, respectively (Slattery et al., 1990). In addition, symmetry boundary conditions were imposed on the plane $z=0$ and axis of symmetry $r=0$.

We used the finite-element method along with the arbitrary Lagrangian–Eulerian method of spines pioneered by Kistler and Scriven (1983) to parametrize the spatial derivatives and the deforming pore interface, following a design that we have successfully applied to similar free-surface flows (Xue et al., 2008; Muddu et al., 2012; Lu and Corvalan, 2012, 2014). The time was discretized using a second-order trapezoidal method with Adam–Bashforth prediction to reduce time truncation errors. To improve computational efficiency, the time steps were calculated using a first-order continuation method (Corvalan and Saita, 1991).

3. Results and discussion

The qualitative behavior of a pore nucleated in a fluid sheet may change substantially with the initial pore size. There are at least four conceivable behaviors: the pore may open, close, flicker or remain stable. Here we discuss three of these scenarios, which are summarized in Fig. 2. The figure compares the time evolution of three different pores which open (long dashed line), close (dashed line), or flicker (solid line) depending solely upon the initial pore size R_0. We have not observed stable pores (in the sense of Taylor and Michael, 1973) for the parameters considered in this paper.

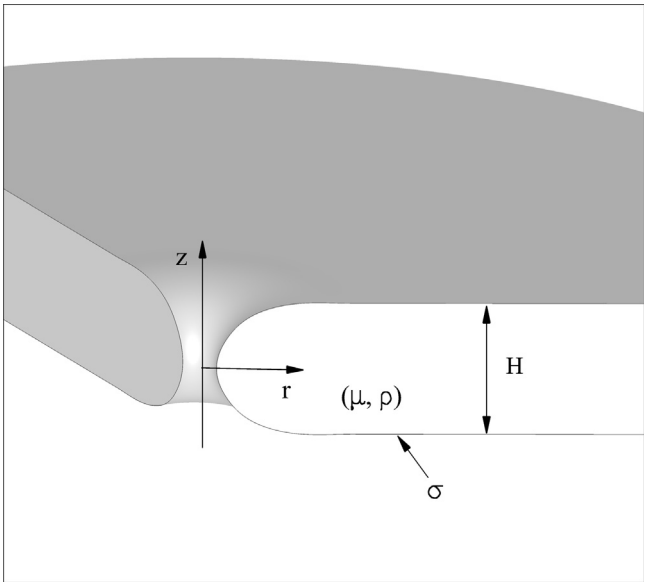

Fig. 1. Small circular pore on a fluid sheet with density ρ, viscosity μ, and surface tension σ. The thickness of the fluid sheet is H and the initial pore radius is R_0.

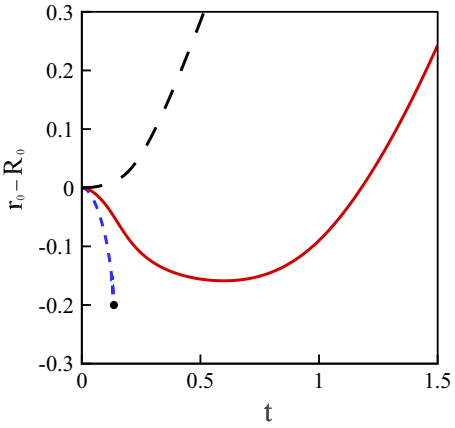

Fig. 2. Influence of initial size on the dynamics of pore formation. Time evolution of the minimum pore radius r_0 in an inertial fluid sheet with $Oh=0.04$. Depending on the initial radius R_0, the pore: (a) expands (long-dashed line, $R_0=50$), (b) contracts (dashed line, $R_0=0.2$), or (c) initially contracts and then expands (solid line, $R_0=0.36$).

3.1. A large expanding pore

Although our focus is on the little-known dynamics of small pores, we begin our discussion with the large opening pore introduced in Fig. 2a in order to make comparisons with a recent work by Savva and Bush (2009). Savva and Bush (2009) investigated in detail the expansion of large pores using a one-dimensional lubrication model in the long wavelength limit. The lubrication model is compared against the full NS solution in Fig. 3, in which we have chosen the parameters to be identical to those used by Savva and Bush (2009) for a large pore in an inertial sheet ($R_0=50$, $Oh=0.04$) to facilitate the comparison.

Despite being a one-dimensional approximation, the lubrication model accurately captures the essential features of the film profile during the expansion of the pore, as shown by directly comparing the profiles from the full NS solutions (solid line) and from the results by Savva and Bush (2009) (circles) in Fig. 3a. As illustrated in the figure, the lubrication model is able to capture not only the formation of the large toroidal rim at the retracting