The propagation of a surfactant laden liquid plug in a capillary tube

S. L. Waters[a] and J. B. Grotberg
Biomedical Engineering Department, University of Michigan, 3304 G G Brown, 2350 Hayward, Ann Arbor, Michigan 48109

(Received 24 October 2000; accepted 14 August 2001)

This paper considers the propagation of a liquid plug, forced by a driving pressure ΔP, within a rigid tube. The tube is already lined with a liquid precursor film of thickness h_2. Both the plug and the precursor film, as well as the interface, contain small amounts of surfactant whose concentrations are assumed to be near equilibrium. Since the motions are slow, we seek asymptotic solutions for small capillary number, $Ca \ll 1$, and also assume that sorption kinetics control the surfactant flux to the interface compared to bulk diffusion. An additional asymptotic assumption is that the Stanton number, *St*, is sufficiently large such that $\beta \propto Ca^{1/3}/St \ll 1$, which relates the importance of sorption kinetics to convection. The surfactant strength is measured by the surface elasticity, $E = M/\beta$ where *M* is the Marangoni number. The results of the analysis are that, for a given plug *Ca*, ΔP increases with increasing *E* but decreases with increasing h_2. The trailing film thickness, h_1, increases with ΔP, but at a slower rate when *E* is larger. For $h_1 < h_2$, criteria for plug rupture are established. This model is relevant to delivery of surfactants into the lung by direct instillation into the bronchial network as is done in surfactant replacement therapy and the use of surfactant solutions to carry other substances (e.g., genetic material) into the airways. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1416496]

I. INTRODUCTION

Pulmonary surfactant reduces the surface tension at the interface between the air within the lung and the thin liquid film lining the airway, thus increasing lung compliance and reducing the amount of work required to expand the lungs with each breath. Surfactant is formed relatively late in fetal development and, as a result, many premature neonates are born with a deficiency of pulmonary surfactant and may suffer from respiratory distress syndrome (RDS). RDS is characterized by low lung compliance, areas of atelectasis, airway closure, poor arterial oxygenation, and fluid filled alveoli. Surfactant replacement therapy (SRT) is now a standard treatment for premature neonates suffering from RDS and has had a dramatic impact on infant survival rate. The most common protocol for instilling surfactant is injecting four quarter dose aliquots into the trachea, although variations of this procedure have been used clinically.[1] Surfactant laden liquid plugs are also used to deliver drugs and genetic materials to normal surfactant lungs.

Halpern, Jensen, and Grotberg[2] and Espinosa and Kamm[3] considered the mechanisms via which a bolus of surfactant spreads to the periphery of the lungs after it has been delivered to the trachea. In the largest airways the liquid plug remains intact and blocks the flow of air along the airways. As it propagates it deposits a trailing film on the airway walls and may eventually rupture; see Howell, Waters, and Grotberg.[4] After rupture, the deposited surfactant rich film then drains under gravity. As it spreads further into the bifurcating airways, the thickness of the film diminishes and gravitational forces become weak compared with surface tension forces. The dominant spreading mechanism is then gradients in surface tension (i.e., Marangoni flows).

Motivated by the clinical application, this paper models the propagation of a surfactant-laden liquid plug along a liquid-lined airway after it has been instilled. The model is most applicable to the later doses of surfactant, as for the initial doses the gradients in surface tension are so large that Marangoni stresses cause the plug to rupture very quickly. The liquid plug propagates along the airway under the pressure drop imposed across it during breathing. Ahead of the plug is a precursor film and as it is pushed through the airway it leaves behind a trailing film, thus coating the airways with a layer of surfactant. Reopening occurs if and when the plug volume decreases to a point at which it ruptures. We model the airway as a liquid-lined, cylindrical rigid tube and assume that the plug propagates in the axial direction along the tube. The thickness of the deposited film and the pressure required to force the plug along the tube will depend on the capillary number, *Ca*, which is the ratio of viscous to surface tension effects. We assume that the motion of the plug is sufficiently slow that the flow is in the Stokes regime and we take *Ca* to be asymptotically small so that surface tension forces are large compared to viscous forces.

There have been a number of theoretical and experimental studies on the low capillary number displacement of a viscous wetting fluid by an inviscid fluid in circular capillaries and between closely spaced flat plates, the results of which are equally applicable to liquid plugs. Experimental work by Fairbrother and Stubbs[5] indicated that the thickness of the liquid lining deposited on the wall of a capillary after

[a]Present address: School of Mathematical Sciences, University of Nottingham, University Park, Nottingham, NG7 2RD, UK. Electronic mail: sarah.waters@nottingham.ac.uk

a wetting viscous fluid is displaced by a gas bubble is proportional to $Ca^{1/2}$ for $10^{-4}<Ca<10^{-2}$. Subsequent work of Taylor[6] confirmed this finding and extended it to higher *Ca*. Marchessault and Mason[7] measured the wetting film thickness in an air–water system experimentally, using a technique based on electrical conductivity, and found for capillary numbers from 10^{-5} to approximately 10^{-4} the results were somewhat larger than those predicted by the Fairbrother–Stubbs correlation. However, none of these results agree with the theoretical results of Bretherton[8] who found that, in the limit of small capillary number, the liquid lining thickness is proportional to $Ca^{2/3}$, work which was later recast in asymptotic form and extended in Park and Homsy;[9] see also Wong, Radke, and Morris.[10,11] Bretherton's experimental work was in good agreement with his theoretical predications for $Ca>10^{-4}$, but for smaller values of *Ca*, where his results should have been more accurate, his theory under-predicted the thickness of the liquid-lining. One theory put forward for the disagreement among the experimental and theoretical results was that small quantities of surface active impurities (surfactants) were present, which may have resulted in the air–liquid interface being able to support a shear stress (surface hardening).

Bretherton[8] and Schwartz, Princen, and Kiss[12] accountable for the influence of surfactants in an *ad hoc* fashion without a detailed account for the surfactant transport mechanism, either by applying the no-slip condition at the interface or by assuming a positive surface tension gradient, i.e., a decrease of surface concentration in the direction of bubble motion. More rigorous analyses of the effects of trace amounts of surfactants on the motion of long gas bubbles in capillaries were carried out by Ginley and Radke[13] and by Ratulowski and Chang.[14] Ginley and Radke assumed that the surfactant concentration in the bulk was uniform and adsorption kinetics was the rate controlling mechanism for the surfactant transport. Their results indicate that, for this particular regime, the surface concentration of surfactant increases in the thin film region compared to the bubble front so that the film thickness decreases compared with the surfactant free case. Ratulowski and Chang carried out a more comprehensive asymptotic analysis for different convective, diffusive and kinetic timescales and they showed that if the transport in the film is mass transfer limited so that a bulk concentration gradient exists in the film, the film thickness increases by a maximum factor of $4^{2/3}$ compared with Bretherton's results at low bubble speeds. Park[15] considered a similar problem for a finite length bubble and showed the film-thickening behavior to be dependent on bubble-length. The effect of surfactant present at elevated concentration on the propagation of a semi-infinite gas bubble in a capillary was considered by Stebe and Barthès-Biesel.[16] The displacement of a wetting fluid by a semi-infinite bubble has also been considered in the context of airway reopening, where now the airway is modeled as a flexible-walled vessel.[17–22]

In our model the fluid contains soluble surfactant which is transported between the bulk phase and the surface. The bulk phase is the liquid region away from the surface, where the surfactant is transported by convection and diffusion. In the region immediately adjacent to the surface (the subsurface phase) the bulk surfactant is in contact with the surface and communicates directly with the surface phase. Additionally, surfactant molecules are adsorbed onto or desorbed from the surface (we neglect the surface diffusivity of surfactant). The flux of surfactant to the surface will be controlled by the slower of the two processes. We assume that the diffusivity of surfactant in the bulk is so large that the bulk concentration of surfactant is constant, so that we do not need to solve the bulk phase transport problem. The transfer of surfactant from the bulk to the surface is controlled by the sorption kinetics. The transport of surfactant along the surface is determined by the relative degree of advection by the flow and the amount of adsorption from the bulk to the surface and *vice versa*. If the adsorption rate were infinite the concentration of surfactant along the surface would be constant and equal to its sorptive equilibrium value. Thus the surface concentration of surfactant would be constant and no gradients in surface tension would exist. In this model we consider perturbations about an infinite adsorption rate and hence introduce Marangoni flows due to surface tension gradients. This is the same parameter regime as studied by Ginley and Radke.[13]

We determine the effect of the imposed pressure drop, surface tension, surface tension gradients and precursor film thickness on the propagation of the liquid plug. In Sec. II we formulate the problem and derive the dimensionless governing equations and parameters. In Sec. III we develop an asymptotic solution for the governing equations in the limit of small capillary number and large adsorption rate. Finally, in Sec. IV we discuss the implications of our results for SRT.

II. FORMULATION

A. Model description

We consider an axisymmetric, impermeable rigid tube of uniform radius a^* lined with an incompressible Newtonian fluid of viscosity μ^*. Throughout this paper stars denote dimensional quantities. A liquid plug of incompressible Newtonian fluid, also of viscosity μ^*, propagates at speed U^* in the axial direction along the tube (see Fig. 1) and separates two semi-infinite fingers of air. The length of the plug is assumed to be of the same order as the tube radius. Since the viscosity of air is much less than the fluid viscosity we assume the air to be inviscid. The fluid contains surfactant which has bulk concentration C_0^* and surfactant molecules are adsorbed onto or desorbed from the interface with rate constants k_1^* and k_2^*, respectively. The sorptive equilibrium surface concentration of surfactant is then $C_0^* k_1^*/k_2^*$ and the corresponding surface tension is σ_0^*.

We consider a cylindrical coordinate system (a^*r, a^*z) with corresponding coordinate directions $(\hat{\mathbf{r}}, \hat{\mathbf{z}})$. The liquid-lining thickness is a^*h so that the position of the air–liquid interface is given by $r=1-h$. The precursor film thickness is a^*h_2 and the trailing film thickness is a^*h_1. The unit normal and unit tangent to the air–liquid interface are denoted by $\hat{\mathbf{n}}$, $\hat{\mathbf{t}}$, respectively, and the interfacial curvature is given by $\mathcal{K}^*=\mathcal{K}/a^*=(\nabla_s\cdot\hat{\mathbf{n}})/a^*$ where $\nabla_s=(\mathrm{I}-\hat{\mathbf{n}}\hat{\mathbf{n}})\cdot\nabla$ is

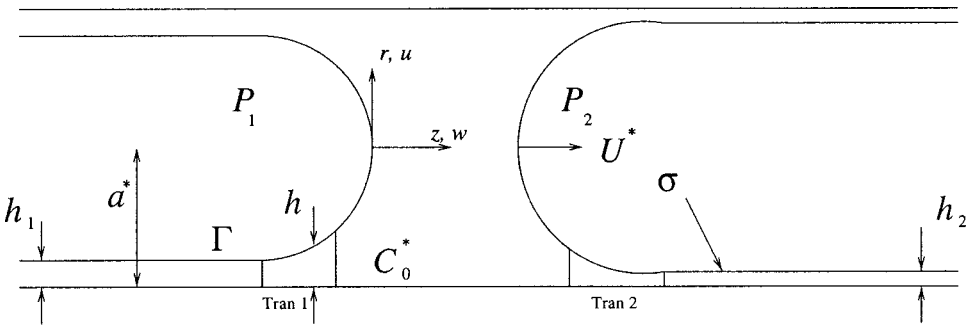

FIG. 1. Definition sketch of the propagating liquid plug.

the surface gradient operator. The fluid velocity is $\mathbf{u}^* = U^*(u,w)$ and $U^*\mathbf{u}_s$ is the surface velocity at the air–liquid interface. The fluid pressure is $(\sigma_0^*/a^*)p$ and $(\sigma_0^*/a^*)\mathbf{s}$ is the stress vector. The air pressures behind and ahead of the liquid plug are $(\sigma_0^*/a^*)(P_1,P_2)$, respectively. Finally, the surface concentration of surfactant is denoted by $a^*C_0^*\Gamma$, the surface tension by $\sigma_0^*\sigma$ and the flux of surfactant to the interface by $C_0^*U^*J$.

B. Dimensionless governing equations and parameters

We assume the plug motion is sufficiently slow that the flow is in the Stokes regime, i.e., we neglect inertia forces, and move to a frame of reference in which the plug is stationary and the walls are moving at (dimensionless) velocity $-\hat{\mathbf{z}}$ with respect to the stationary plug. We also neglect buoyancy effects. The dimensionless fluid dynamic equations are the continuity and Stokes equations

$$\nabla\cdot\mathbf{u}=0, \tag{1a}$$

$$\nabla p=\tfrac{1}{3}Ca\nabla^2\mathbf{u}, \tag{1b}$$

where $Ca=3\mu^*U^*/\sigma_0^*$ is the capillary number and is the ratio of the viscous to surface tension forces (the factor of three here is introduced for later convenience).

The equation governing the transport of surfactant along the interface is

$$-\frac{\partial\Gamma}{\partial z}+\nabla_s\cdot(\Gamma(\mathbf{u}_s+\hat{\mathbf{z}}))=J, \tag{2}$$

so that advection of surfactant along the surface is balanced by the sorptive flux. We have neglected surface diffusivity in this analysis. Agrawal and Neuman[23] measured the surface diffusivity, D_s^*, of DPPC (the main lipid component of pulmonary surfactant) in myristic acid and found $10^{-7}<D_s^*<7\times10^{-5}$ cm^2/s. Assuming that $\mu^*\approx10^{-2}$ g/cms, $\sigma_0^*\approx10$ dyn/cm and $a^*h\approx10$ μm the surface diffusivity term is $\mathcal{O}(\mu^*D_s^*/\sigma_0^*a^*h)\sim\mathcal{O}(10^{-4})$ compared with the advection term and hence we are justified in neglecting surface diffusivity.

The boundary conditions for the fluid motion are

$$\mathbf{u}=-\hat{\mathbf{z}} \quad \text{at } r=1\,(\text{tube wall}), \tag{3a}$$

$$\left.\begin{aligned}&\hat{\mathbf{t}}\cdot\mathbf{s}=\hat{\mathbf{t}}\cdot\nabla_s\sigma \qquad (3b)\\ &\mathbf{s}\cdot\hat{\mathbf{n}}=-\sigma\mathcal{K}-P_a \qquad (3c)\\ &\frac{D}{Dt}(r+h)=0 \qquad (3d)\end{aligned}\right\} \quad \text{at } r=1-h\,(\text{air–liquid interface}),$$

where $\mathbf{s}=-p\hat{\mathbf{n}}+\frac{1}{3}Ca\,\tau\cdot\hat{\mathbf{n}}$ and τ is the dimensionless stress tensor. Equation (3a) is the no-slip boundary condition. Equations (3b) and (3c) are the tangential and normal stress conditions at the interface while (3d) is the kinematic boundary condition. In Eq. (3c) P_a denotes the air pressure ($P_a=P_1$ behind the plug and P_2 ahead of the liquid plug). In order to determine the axial boundary conditions, we assume that in the laboratory frame there is no flow at $z=\pm\infty$, the flat film regions. Thus in the plug frame of reference, the dimensionless upstream and downstream conditions are

$$\mathbf{u}\to-\hat{\mathbf{z}} \ \text{ as } \ z\to\pm\infty. \tag{4}$$

This limiting velocity boundary condition must be accompanied by a compatible limiting condition for the interfacial surfactant concentration since a flat velocity profile can only exist in a flat film if the surface tension gradient, caused by a surfactant concentration gradient, is absent.

The flux of surfactant from the bulk to the interface is controlled by the sorption kinetics, with J as follows:

$$J=St\left(1-\frac{\Gamma}{K}\right), \tag{5}$$

where $St=k_1^*/U^*$ is the Stanton number and is the ratio of the time scale of the flow to the time scale for adsorption and $K=k_1^*/k_2^*a^*$ is the adsorption equilibrium constant, thus $\Gamma=K$ is the (dimensionless) sorptive equilibrium surface surfactant concentration. Physically K may be thought of as the depth into the bulk-phase that would contain the same number of surfactant molecules per unit area as found at the surface, at equilibrium. The axial boundary conditions for Γ are

$$\Gamma\to K \ \text{ as } \ z\to\pm\infty. \tag{6}$$

Note that these boundary conditions do not imply that the entire air–liquid interface far away from the plug has a surfactant concentration in equilibrium with the bulk surfactant

concentration in the plug. The lengthscale of these far away boundary conditions is a few plug lengths. The maximum distance is of the order of an airway length, since at distances greater than this the next airway is reached and the conditions are different.

Finally we need an equation of state relating the surface tension to the surface concentration of surfactant. Since we shall be considering small deviations of the surface surfactant concentration from its sorptive equilibrium value we use a linearized equation of state:

$$\sigma = 1 - M(\Gamma - K), \tag{7}$$

where

$$M = -\left(\frac{\partial \sigma}{\partial \Gamma}\right)\bigg|_{\Gamma = K}, \tag{8}$$

is the Marangoni number and represents the ability of the surfactant to modify the surface tension from the equilibrium value.

III. ASYMPTOTIC SOLUTION

Numerical attempts to solve the much simpler surfactant free problem have had some success for limited parameter ranges.[24–26] As an alternative we seek approximate solutions to the governing equations by undertaking an asymptotic analysis similar to that of Howell, Waters, and Grotberg[4] for the surfactant free problem.

Since the motion of the plug is slow, the capillary number is very small ($Ca \ll 1$). We thus consider an asymptotic expansion for the dependent variables in powers of the capillary number, retaining only leading order terms. The transport of surfactant along the interface is governed by St [(2) and (5)]. We are concerned with perturbations of the surfactant concentration from equilibrium that correspond to $St \gg Ca^{1/3}$. This is the bulk equilibrium model described in Ratulowski and Chang.[14] Thus we consider a second perturbation expansion in powers of $1/\hat{\beta}$ where $\hat{\beta} = St/Ca^{1/3} \gg 1$. We will expect the leading order surface surfactant concentration to be $\Gamma = K$. The Marangoni number, M, is $\mathcal{O}(1)$ throughout.

A. Quasi-steady solution for the menisci

Since Ca is the smallest parameter of the problem we consider a regular perturbation expansion of the dependent variables in powers of Ca. From (1b) at leading order we have that

$$\nabla p = 0, \tag{9}$$

so that the plug pressure is constant. Hence, at low Ca, we expect the menisci on either side of the plug to the approximately static spherical caps. The surfactant equation (2) gives that $\Gamma = K$ at leading order so that the concentration is constant and equal to the sorptive equilibrium value. Thus we have no Marangoni effects in this region at this order.

Suppose we define the pressure drop across the rear meniscus, ΔP_1, to be

$$\Delta P_1 = -p + P_1, \tag{10}$$

and the position of the interface to be $r = R(z)$. We choose $z = 0$ to be the longitudinal position at which the rear meniscus intersects the tube axis. The shape of the interface may then be determined by integrating the normal stress balance, (3c), to give

$$R(z) = \frac{2}{\Delta P_1}\left\{1 - \left(\frac{\Delta P_1}{2} z + 1\right)^2\right\}^{1/2}, \tag{11}$$

which is valid up to $\mathcal{O}(Ca)$. The shape of the front interface may be determined similarly. It is also convenient to define here the pressure drop across the front meniscus, ΔP_2, and the pressure drop across the plug, ΔP, respectively, as

$$\Delta P_2 = -p + P_2, \quad \Delta P = \Delta P_1 - \Delta P_2. \tag{12}$$

B. Lubrication analysis

A spherical cap (11) cannot be smoothly joined to the uniform thin film regions upstream and downstream of the plug. Therefore, transition regions are required in which the viscous forces and the Marangoni stresses arising due to surface tension gradients are as important as the effect of surface tension. These regions are marked Tran 1 and Tran 2 in Fig. 1. In the transition regions the liquid layer is thin, with a slowly varying free surface, so we can use lubrication theory. We rescale as follows:[4,8,14,15]

$$r = 1 - Ca^{2/3}\overline{y}, \tag{13a}$$

$$z + l = Ca^{1/3}\overline{z}, \tag{13b}$$

$$(h, h_1) = Ca^{2/3}(\overline{h}, \overline{h_1}), \tag{13c}$$

$$\Gamma = Ca^{2/3}\overline{\Gamma}, \tag{13d}$$

$$K = Ca^{2/3}\overline{K}, \tag{13e}$$

$$u = Ca^{1/3}\overline{u}, \tag{13f}$$

$$w = \overline{w}, \tag{13g}$$

where $z = -l$ is the origin of the coordinate system for the transition region. The rescaling (13d) is necessary so that the Marangoni effects enter the surfactant transport equation at leading order. Hence the validity of the analysis is restricted to special cases in which only trace amounts of surfactant is present. In order to simplify the analysis we take $\overline{K} \equiv 1$.

We start by considering the rear transition region (Tran 1 in Fig. 1). If the above scalings are substituted into Eqs. (1)–(7) and we neglect terms that are $O(Ca^{1/3})$ compared with the leading order terms we can derive the following coupled ordinary differential equations for the film thickness, h, and the surfactant concentration, Γ:

$$-\overline{h}^3\overline{h}_{\overline{zzz}} + \tfrac{3}{2}M\overline{\Gamma}_{\overline{z}}\overline{h}^2 + \overline{h} - \overline{h}_1 = 0, \tag{14a}$$

$$\frac{\partial}{\partial \overline{z}}\left(\overline{\Gamma}\left(\frac{3}{2}\overline{h}_{\overline{zzz}}\overline{h}^2 - 3M\overline{\Gamma}_{\overline{z}}\overline{h} - 1\right)\right) = \hat{\beta}(1 - \overline{\Gamma}). \tag{14b}$$

The equations are transformed into canonical form for numerical integration

$$-H^3H_{ZZZ}+\frac{3}{2}M\overline{\Gamma}_Z H^2+H-\frac{\overline{h}_1}{\overline{h}_1^0}=0, \tag{15a}$$

$$\frac{\partial}{\partial Z}\left(\overline{\Gamma}\left(\frac{3}{2}H_{ZZZ}H^2-3M\overline{\Gamma}_Z H-1\right)\right)=\beta(1-\overline{\Gamma}), \tag{15b}$$

using

$$H=\frac{\overline{h}}{\overline{h}_1^0}, \tag{16a}$$

$$\overline{z}+s=\overline{h}_1^0 Z, \tag{16b}$$

$$\beta=\overline{h}_1^0\hat{\beta}, \tag{16c}$$

where $\overline{h}_1^0$ is the constant trailing film thickness for a bubble at constant sorptive equilibrium surface tension and s is an arbitrary shift of coordinates.

We consider an asymptotic expansion for H and $\overline{\Gamma}$ of the form

$$H=H^0+\frac{1}{\beta}H^1+\cdots, \tag{17a}$$

$$\overline{\Gamma}=\overline{\Gamma}^0+\frac{1}{\beta}\overline{\Gamma}^1+\cdots, \tag{17b}$$

so at leading order Eqs. (15a) and (15b) become

$$H^0_{ZZZ}=\frac{H^0-1}{H^{0^3}}, \tag{18a}$$

$$\overline{\Gamma}^0=1. \tag{18b}$$

Equation (18a) is the Landau–Levich equation while (18b) gives that the leading order surfactant concentration is constant, as expected.

At first order the following equations are obtained (where $H^1=M\hat{H}$ for convenience):

$$\hat{H}_{ZZZ}=\frac{\hat{H}(-2H^0+3)-\hat{B}H^0-\frac{9}{4}(H^0H^0_{ZZ}-2H^{0^2}_Z)}{H^{0^4}}, \tag{19a}$$

$$\overline{\Gamma}^1=-\frac{3}{2}\frac{H^0_Z}{H^{0^2}}, \tag{19b}$$

and $\hat{B}=1/M\overline{h}_1^1/\overline{h}_1^0$. Hence, at first order in $1/\beta$ we introduce gradients in surface surfactant concentration, and hence surface tension gradients.

We solve (18a) and (19a) numerically with boundary conditions obtained from the asymptotic behavior at $Z\to\pm\infty$, in a manner similar to Howell, Waters, and Grotberg.[4] For example, an initial condition on (18a) is that the film becomes uniform far away from the plug. We linearize Eq. (18a) by substituting

$$H^0\sim 1+\epsilon e^{\lambda Z} \quad \text{where} \quad \epsilon\ll 1. \tag{20}$$

The eigenvalue λ solves the cubic polynomial

$$\lambda^3-1=0, \tag{21}$$

which has one positive real root and two complex roots with negative real part. To ensure that the uniform film is approached as $Z\to-\infty$, we choose as our initial condition the exponentially decaying eigenfunction. This one initial condition specifies the problem up to an arbitrary translation in Z, so that the value of s is set by the choice of ϵ. The solution to (19a) is found similarly.

The solutions for (18a) and (19a) behave quadratically for large, positive Z

$$H^0\sim\tfrac{1}{2}D_0Z^2+D_1Z+D_2, \tag{22a}$$

$$\hat{H}\sim\tfrac{1}{2}E_0Z^2+E_1Z+E_2 \quad \text{as} \quad Z\to\infty, \tag{22b}$$

where D_0, D_1, D_2, and E_0, E_1, E_2 are numerically determined constants. Once the film thickness in the transition region has been determined it is straightforward to compute the perturbation to the surfactant concentration using Eq. (18b).

The transition region solution is then matched with the quasi-steady solution of Sec. III A

$$\lim_{z\to-l}R(z)=\lim_{\overline{z}\to\infty}(1-Ca^{2/3}\overline{h}). \tag{23}$$

Following Park and Homsy (1984),[9] we observe that since the origin of the transition region coordinate system is moving with the interface, we can anticipate that l is not a function of Ca. Hence l has only one superscript that represents the order of $1/\beta$

$$l=l^0+\frac{1}{\beta}l^1+\cdots. \tag{24}$$

In order that the spherical cap matches the free surface displacement in the transition region the equation of the spherical cap, $R(z)$, and the pressure drop, ΔP_1, must be of the form

$$(R(z),\Delta P_1)=\sum_{n,m}Ca^{n/3}\frac{1}{\beta^m}(R^{nm},\Delta P_1^{nm}), \tag{25}$$

where the first superscript refers to the power of $Ca^{1/3}$ and the second superscript to the power of $1/\beta$. The trailing film thickness and the pressure drop are then determined from the matching conditions at each order.

The trailing film thickness, h_1, and the pressure drop, ΔP_1, are given by

$$\begin{aligned} h_1&\sim 0.643Ca^{2/3}(1-0.0157E),\\ \Delta P_1&\sim 2(1+1.8Ca^{2/3}+0.4E\ Ca^{2/3}), \end{aligned} \tag{26}$$

where $E=M/\beta$ is referred to as the elasticity constant and is an indication of the degree of surfactant activity. These results are in agreement with Ginley and Radke.[13] When $E=0$ we thus recover Bretherton's constant surface tension solution,[8] which indicates that the trailing film thickness and the pressure drop across the rear meniscus increase as the capillary number increases. The surface tension gradients, introduced at $\mathcal{O}(1/\beta)$, result in a decrease in the trailing film thickness. However, the effect is small; when $E=1$ the film thickness decreases by ≈1%. However, the surface tension gradients result in a large increase in the pressure drop across

the rear meniscus, the ratio of ΔP_1^{21} to ΔP_1^{20} is ≈ 0.2 when $E=1$ and the contribution to the total pressure drop from ΔP_1^{21} increases as E increases.

The same asymptotic arguments are applied to the front of the plug. The governing equations for the front transition region are as before [(18a), (18b), (19a), and (19b)] with H now defined by $H=h/\bar{h}_2^0$ and $\hat{B}$ by $\bar{h}_2^1/(\bar{h}_2^0 M)$ and are once again solved in a similar way to the methods detailed in Howell, Waters, and Grotberg.[4] The initial conditions of uniform H are now imposed for large positive Z. Since (21) possesses two roots with negative real part, this problem admits a one parameter family of solutions. The initial condition on (18a) is of the form

$$H^0 = 1 + \epsilon_1 e^{-(1/2)Z} \cos\frac{\sqrt{3}}{2} Z \quad \text{as} \quad Z \to \infty, \tag{27}$$

where ϵ_1 is an arbitrary constant which parameterizes the solution space. Once again we expect the transition region film thickness to behave quadratically as it approaches the meniscus so

$$H^0 \sim \tfrac{1}{2}\hat{D}_0 Z^2 + \hat{D}_1 Z + \hat{D}_2 \quad \text{as} \quad Z \to -\infty. \tag{28}$$

Matching, as before, gives

$$\hat{D}_0 = \bar{h}_2^0. \tag{29}$$

However, in this case $\bar{h}_2^0$ is a physically specified quantity, i.e., (29) is an equation for $\hat{D}_0$. The method employed to solve this problem is as follows: Equation (27) is used as an initial condition to solve (18a) as an initial value problem, with ϵ_1 a shooting parameter to be adjusted until (29) is satisfied. Once the leading order solution, H^0, has been determined, the higher order equations are solved in a similar way.

The pressure drops across the front meniscus is also found by matching. Once this is found, we are then able to compute the pressure drop across the plug. Note that the length of the plug plays no part in our analysis. This is a result of our implicit assumption that the plug length is the same order as the tube radius. If the plug is much longer, viscous drag contributes to the pressure drop across the plug. On the other hand if the plug is short, then the interaction between the two menisci must be accounted for.

C. Results

Ginley and Radke[13] considered the same equations [(18a), (18b), (19a), and (19b)] when analyzing the influence of soluble surfactants on the flow of long bubbles through a circular cylinder. However, the boundary conditions for this problem are different since the precursor film thickness, $\bar{h}_2$, is specified. Here, the total pressure drop, ΔP, across the plug depends on the precursor film thickness, $\bar{h}_2$, the capillary number, Ca, and the elasticity constant, E. Thus, if ΔP, $\bar{h}_2$, and E are specified, we can determine the corresponding plug propagation speed, given by Ca. Since many of the plug properties depend on Ca we can thus investigate their variation with the parameters of the system.

In Fig. 2, the total pressure drop across the plug is plotted as a function of the precursor film thickness, i.e., we plot $\Delta P/Ca^{2/3}$ versus $\bar{h}_2$. Three value of E are considered. For fixed E, the total pressure drop across the plug decreases as $\bar{h}_2$ increases. As E increases, the total pressure drop across the plug, for a given $\bar{h}_2$, increases. Thus, the surface tension gradients result in an increase of the total pressure drop across the plug so that it is harder to force the plug along the tube.

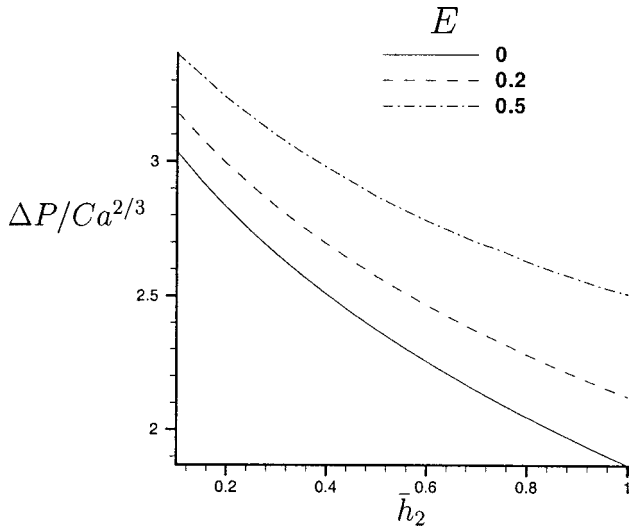

FIG. 2. Total dimensionless pressure drop across the plug as a function of the precursor film thickness $\bar{h}_2$. $E=0$, 0.2, 0.5.

In Fig. 3 we plot the air–liquid interface positions as a function of the pressure drop, ΔP, for various values of $\bar{h}_2$ and E. In all cases, as ΔP increases the capillary number increases so that the film thickness increases. In Fig. 3(a), corresponding to $\bar{h}_2=1$ and $E=0$, the trailing film thickness is less than the precursor film thickness, so that as the plug propagates it picks up more fluid than it deposits and the plug, therefore, grows in size. In Fig. 3(b), corresponding to $\bar{h}_2=0.5$ and $E=0$, we have the opposite situation and the plug shrinks in size as it propagates. In Figs. 3(c) and 3(d) the elasticity parameter $E=1$. The film height is much less than the corresponding situations when $E=0$. Increasing E means that it is harder to force the plug through the tube so that for a given pressure drop the capillary number significantly decreased, and thus the film height decreases.

In Fig. 4(a), the trailing film thickness, h_1 is plotted as a function of the total pressure drop, ΔP, for three values of E. As ΔP increases, for fixed values of E, the trailing film thickness increases, corresponding to an increase in the plug propagation speed. Increasing E results in a decrease in the trailing film thickness. Two factors contribute to this decrease in h_1. First, for a fixed capillary number the trailing film thickness decreases as E increases [see (26)]. Second, as E increases it is harder to force the plug through the tube so that the capillary number, corresponding to a given ΔP, decreases and, since $h_1 \sim Ca^{2/3}$, the trailing film thickness thus decreases. The second factor has the greatest influence on the trailing film thickness.

The rate at which the plug volume, V^*, changes is given to leading order by[4]

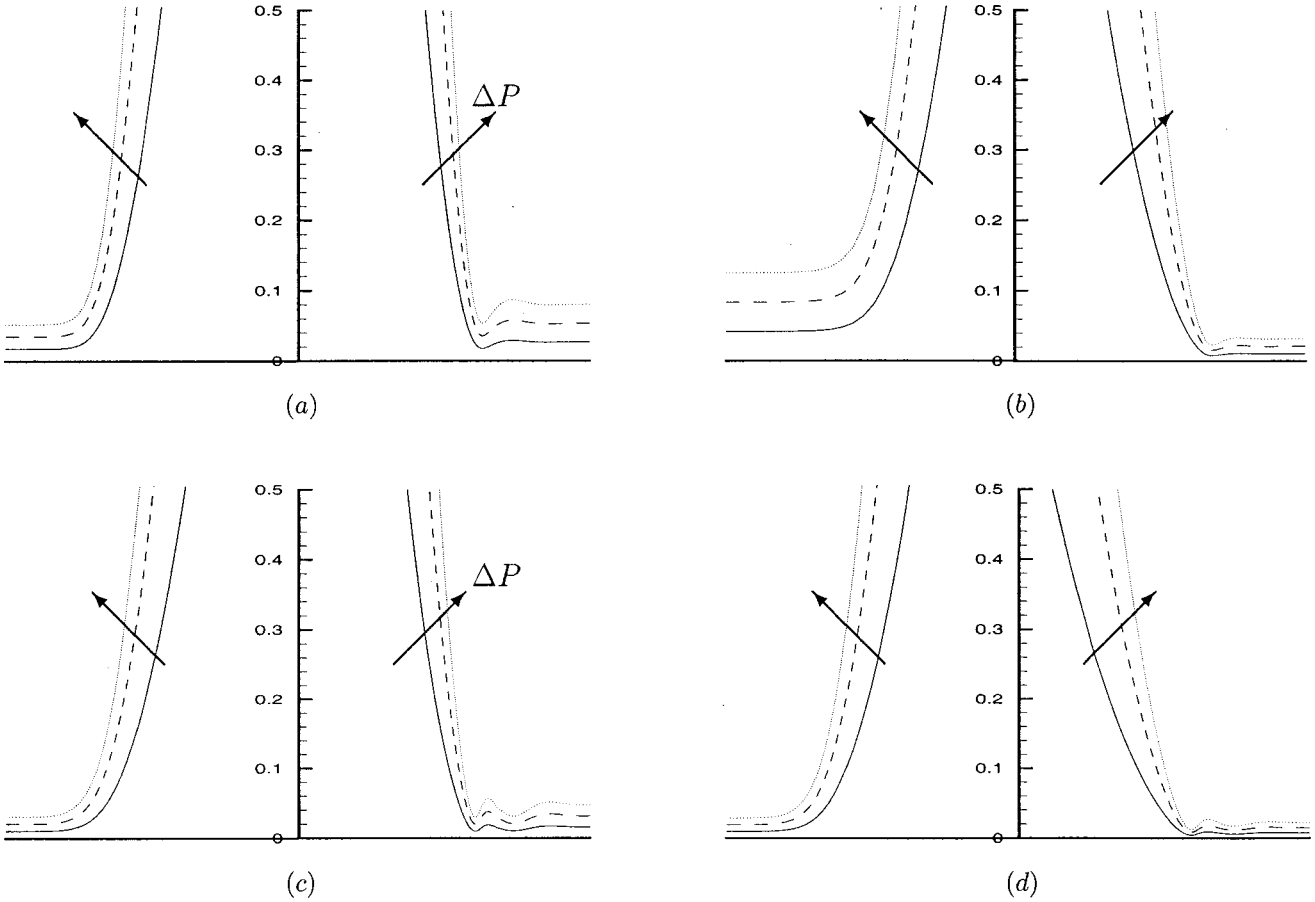

FIG. 3. Solution for the film height ahead and behind the plug. $\Delta P=0.1, 0.2, 0.3$. (a) $\overline{h_2}=1$, $E=0$; (b) $\overline{h_2}=0.5$, $E=0$; (c) $\overline{h_2}=1$, $E=1$; (d) $\overline{h_2}=0.5$, $E=1$. Solid: $\Delta P=0.1$; dashed: $\Delta P=0.2$; dotted: $\Delta P=0.3$.

$$\frac{dV^*}{dt^*}\sim 2\pi a^{*2}U^*(h_2-h_1), \tag{30}$$

which, nondimensionalized gives the dimensionless volume rate, Q,

$$Q=\frac{dV}{dt}\sim Ca(h_2-Ca^{2/3}\overline{h_1})=Ca^{5/3}(\overline{h_2}-\overline{h_1}). \tag{31}$$

The volume rate is plotted as a function of Ca in Fig. 4(b) for two different values of the precursor film thickness

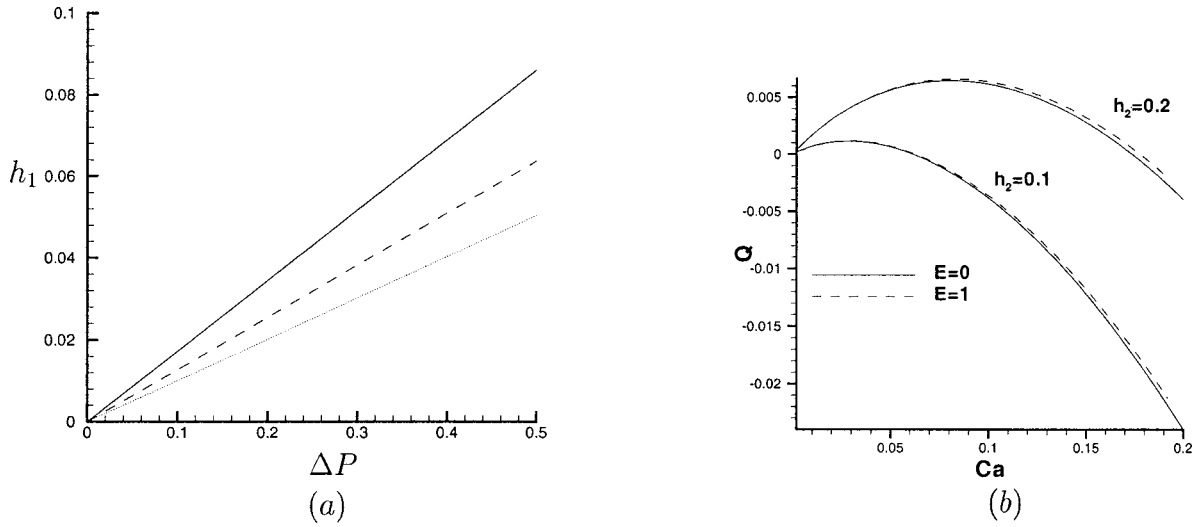

FIG. 4. (a) Trailing film thickness, h_1, versus pressure drop, ΔP. $E=0, 0.5, 1.0$. (b) Volume rate as a function of the capillary number.

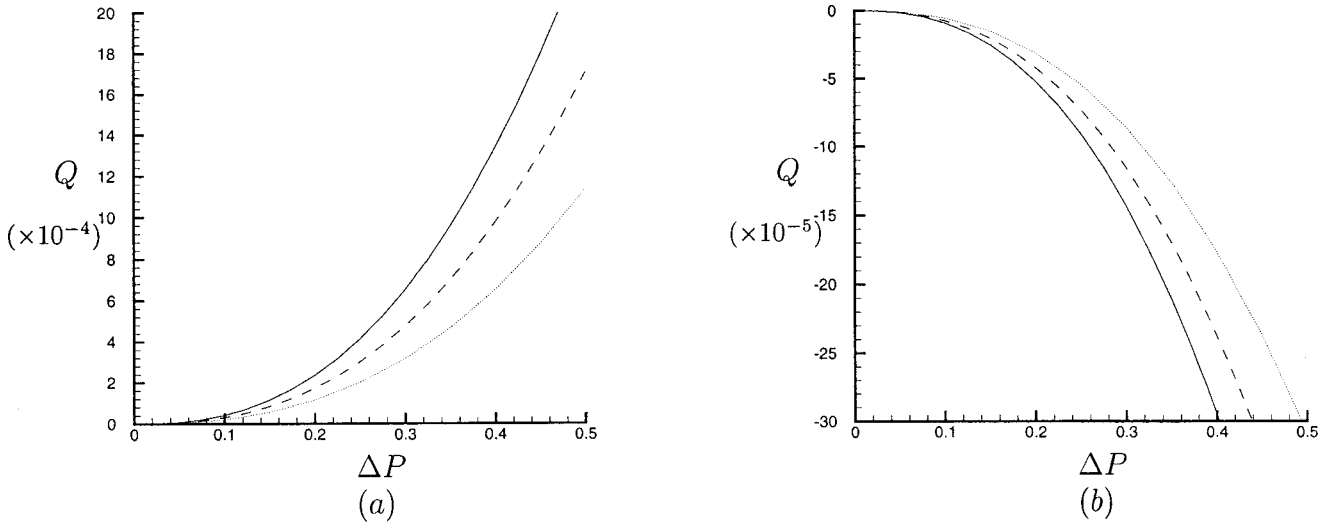

FIG. 5. Volume rate as a function of the pressure drop, ΔP. Solid: $E=0$; dashed: $E=0.2$; dotted: $E=0.5$. (a) $\bar{h}_2=1$; (b) $\bar{h}_2=0.5$.

h_2. As h_2 increases the volume rate, at a given value of Ca, increases. As E increases, the volume rate also increases as the amount of fluid that is being deposited on the trailing film decreases. Note, however, that the effect is very small compared to the effect of changing the precursor film thickness.

In each case in Fig. 4(b) there is a value of Ca where the volume rate changes from being positive (corresponding to the plug volume increasing), to being negative (plug volume decreasing). This we refer to as the critical capillary number, Ca_c, for rupture. It can clearly be seen that as E increases the critical reopening capillary number increases, but the effect is slight (as expected since the effect of varying E on the deposited trailing film thickness is small).

The volume rate is plotted as a function of ΔP in Fig. 5 for three values of E. Two different values of the precursor film thickness, h_2, are considered. In Fig. 5(a), corresponding to $\bar{h}_2=1$, the precursor film thickness exceeds the trailing film thickness. Hence the plug grows as it propagates along the channel so that Q is positive. Increasing E results in a decrease in the volume flow rate, for a given ΔP; despite the fact that $\bar{h}_1$ decreases as E increases, the dominant effect of increasing E is to reduce the propagation speed of the plug significantly and it is this effect that results in Q decreasing. In Fig. 5(b), corresponding to $\bar{h}_2=0.5$, the precursor film thickness is less than the trailing film thickness, and the plug shrinks as it propagates (corresponding to $Q<0$).

Finally in Fig. 6 the volume rate is plotted as a function of ΔP for two different values of the overall precursor film thickness $h_2=0.1,\ 0.15$, and two different values of E. As h_2 increases (for fixed E), the volume rate, at a given value of ΔP, increases. In each case there is a value of ΔP where the flow rate changes from being positive to being negative. This we refer to as the critical reopening pressure, ΔP_c, for rupture. It can clearly be seen that as h_2 and E increase ΔP_c increases. However, whereas the effect of E on the critical reopening capillary number is slight [see Fig. 4(b)] E significantly increases the critical reopening pressure for rupture.

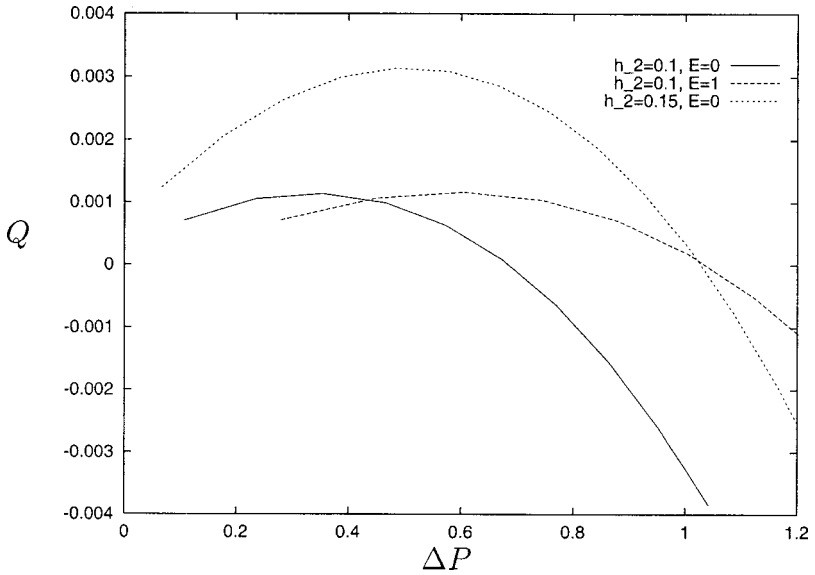

FIG. 6. Volume rate as a function of the pressure drop, ΔP.

IV. DISCUSSION

We have shown that trace amounts of surfactant can significantly affect the dynamics of a liquid plug as it propagates along a rigid, liquid lined tube. The important dimensionless governing parameters are the capillary number, Ca, the pressure drop, ΔP, the elasticity parameter, $E=M/\beta$, and the precursor film thickness, $\bar{h}_2$.

As surfactant is added to the system the value of the sorptive equilibrium surface tension, σ_0^*, decreases and hence the capillary number $Ca \propto \sigma_0^{*-1}$ and the elasticity parameter $E \propto \sigma_0^{*-1/3}$ increase (for a given plug velocity, U^*). Thus since the pressure drop across the plug and the trailing film thickness are proportional to $Ca^{2/3}$, the leading order effect of adding surfactant is to increase the pressure drop required to force the plug through the tube at a given velocity and to increase the thickness of the deposited trailing film.

Suppose now that we fix the capillary number. Then as E increases (for example, via an increase in the Marangoni number) the pressure drop across the plug required to maintain a given plug velocity increases while the trailing film thickness decreases slightly.

We discuss now the implications of these results for SRT. There are a number of clinical problems associated with surfactant replacement therapy. If the plug ruptures too quickly the surfactant will not reach many of the smaller airways. On the other hand, one of the problems encountered by clinicians is that surfactant gets blown out of the lung during expiration, and we propose that this may be due to incomplete delivery (the plug never ruptured) or the formation of trailing plugs. It is, therefore, desirable that the plug ruptures in the time between two breaths, to prevent the plug from being blown out during exhalation. Thus one of the questions facing clinicians is: What is the optimum method to deliver surfactant which avoids either of these problems? (For a discussion of liquid plug behavior in the absence of surfactant see Halpern, Jensen, and Grotberg.[2])

One feature of the treatment that clinicians can control is the quantity of surfactant that is administered in each dose. If a large amount of surfactant is added in one dose then there will be a large increase in the capillary number accompanied by an increase in the value of E. However, the effects of surface tension gradients will be small compared to the effect of increasing the capillary number. Increasing the capillary number is likely to push the plug into the rupture regime, corresponding to the volume rate being negative; see Fig. 4(b). Since the effect of nonzero E is to increase the critical capillary number required for rupture only slightly it will not be able to compensate the large effect due to the increase in capillary number. There are two further adverse effects associated with increasing the capillary number too rapidly. First, the thickness of the trailing film will increase which may lead to the formation of trailing plugs through the Rayleigh instability. Second, as the capillary number increases the pressure drop required to maintain the plug velocity increases rapidly, so that the amount of work required to force the plug through the airways increases.

If, alternatively, a smaller amount of surfactant is added in one dose then the resulting increase in capillary number is smaller and hence the effects of surface tension gradients are more significant and plug rupture is less likely allowing surfactant to be distributed further into the airways. Thus a large dose of surfactant is more likely to rupture quickly preventing delivery of exogenous surfactant to the smaller airways.

ACKNOWLEDGMENTS

The authors would like to thank Dr. David Halpern and Dr. Graeme Keith for many helpful discussions and for their careful reading of the manuscript. This work was supported by NIH Grant No. HL41126, NSF Grants No. BES-9820967 and No. CTS-9412523, and NASA Grant No. NAG3-2196.

[1] E. M. Zola, A. M. Overbach, J. H. Gunkel, R. K. Chan, M. O. Lim, I. Knox, B. H. Feldman, S. E. Denson, B. S. Stonestreet, B. R. Mitchell, M. W. Wyza, K. J. Bennett, and A. J. Gold, "Comparison of three dosing procedures for administration of bovine surfactant with respiratory distress syndrome," J. Pediatr. **122**, 453 (1993).
[2] D. Halpern, O. E. Jensen, and J. B. Grotberg, "A theoretical study of surfactant and liquid delivery into the lung," J. Appl. Physiol. **85**, 333 (1998).
[3] F. F. Espinosa and R. D. Kamm, "Bolus dispersed through the lungs in surfactant replacement therapy," J. Appl. Physiol. **86**, 391 (1999).
[4] P. D. Howell, S. L. Waters, and J. B. Grotberg, "The propagation of a liquid bolus along a liquid-lined tube," J. Fluid Mech. **406**, 309 (2000).
[5] E. Fairbrother and A. E. Stubbs, "Studies in electroendosmosis. Part VI. The 'bubble-tube' methods of measurement," J. Chem. Soc. Lond. **1**, 527 (1935).
[6] G. I. Taylor, "Deposition of a viscous fluid on the wall of a tube," J. Fluid Mech. **10**, 161 (1961).
[7] R. N. Marchessault and S. G. Mason, "Flow of entrapped bubbles through a capillary," Ind. Eng. Chem. **52**, 79 (1960).
[8] F. P. Bretherton, "The motion of long bubbles in tubes," J. Fluid Mech. **10**, 166 (1961).
[9] C.-W. Park and G. M. Homsy, "Two-phase displacement in Hele Shaw cells: theory," J. Fluid Mech. **139**, 291 (1984).
[10] H. Wong, C. J. Radke, and S. Morris, "The motion of long bubbles in polygonal capillaries. Part 1. Thin films," J. Fluid Mech. **292**, 71 (1995).
[11] H. Wong, C. J. Radke, and S. Morris, "The motion of long bubbles in polygonal capillaries. Part 2. Drag, fluid pressure and fluid flow," J. Fluid Mech. **292**, 95 (1995).
[12] L. W. Schwartz, H. M. Princen, and A. D. Kiss, "On the motion of bubbles in capillary tubes," J. Fluid Mech. **172**, 259 (1986).
[13] G. M. Ginley and C. J. Radke, "The influence of soluble surfactants on the flow of long bubbles through a cylindrical capillary," ACS Symp. Ser. **369**, 480 (1989).
[14] J. Ratulowski and H.-C. Chang, "Marangoni effects of trace impurities on the motion of long gas bubbles in capillaries," J. Fluid Mech. **210**, 303 (1990).
[15] C.-W. Park, "Influence of soluble surfactants on the motion of finite bubble in a capillary tube," Phys. Fluids A **4**, 2335 (1992).
[16] K. J. Stebe and D. Bathés-Biesel, "Marangoni effects of adsorption-desorption controlled surfactants on the leading end of an infinitely long bubble in a capillary," J. Fluid Mech. **286**, 25 (1995).
[17] D. P. Gaver, D. Halpern, O. E. Jensen, and J. B. Grotberg, "The steady motion of a semi-infinite bubble through a flexible-walled channel," J. Fluid Mech. **319**, 25 (1996).
[18] D. P. Gaver, R. W. Samsel, and J. Solway, "Effects of surface tension and viscosity on airway reopening," J. Fluid Mech. **319**, 25 (1990).
[19] S.-H. Hsu, K. P. Strohl, M. A. Haxhiu, and A. M. Jamieson, "Role of viscoelasticity in the tube model of airway reopening. II. Non-Newtonian gels and airway simulation," J. Appl. Physiol. **80**, 1649 (1996).
[20] M. L. Perun and D. P. Gaver, "An experimental model investigation of the opening of a collapsed untethered pulmonary airway," J. Biomech. Eng. **117**, 1 (1995).

[21]S. N. Ghadiali and D. P. Gaver, ''An investigation of pulmonary surfactant physiochemical behavior under airway reopening conditions,'' J. Appl. Physiol. **88**, 493 (2000).
[22]D. Y. K. Yap and D. P. Gaver, ''The influence of surfactant on two-phase flow in a flexible-walled channel under bulk equilibrium conditions,'' Phys. Fluids **10**, 1846 (1998).
[23]M. L. Agrawal and R. D. Neuman, ''Surface diffusion in monomolecular films. II. Experiment and theory,'' J. Colloid Interface Sci. **121**, 366 (1988).
[24]W. Q. Lu and H.-C. Chang, ''An extension of the biharmonic boundary integral method to free surface flow in channels,'' J. Comp. Physiol. **77**, 340 (1988).
[25]D. A. Reinelt and P. G. Saffman, ''The penetration of a finger into a viscous fluid in a channel and a tube,'' SIAM (Soc. Ind. Appl. Math.) J. Sci. Stat. Comput. **6**, 542 (1985).
[26]E. I. Shen and K. S. Udell, ''A finite element study of low Reynolds number two-phase flow in cylindrical tubes,'' J. Appl. Mech. **107**, 253 (1985).