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Thin-film dynamics above a periodically-stretched alveolar substrate

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THIN-FILM DYNAMICS ABOVE A PERIODICALLY-STRETCHED ALVEOLAR SUBSTRATE

BY

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Bachelor of Engineering, University of Science and Technology of China (2004)

THESIS

Submitted to the University of New Hampshire in partial fulfillment of the requirements for the degree of

Master of Science in Mechanical Engineering

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08/21/67
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Dedication

To my beloved Dad and Mom for their continuing support.
Acknowledgments

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Summary of dominant physical processes in different regions of $A-\omega$ parameter space investigated in this study.
ABSTRACT
THIN-FILM DYNAMICS ABOVE A PERIODICALLY-STRETCHED ALVEOLAR SUBSTRATE

by
Lu Luo
University of New Hampshire, September, 2007

During last few years several new respiratory diseases including SARS and avian flu have appeared in various parts of the world. With deteriorating environmental conditions and increased air travel, more and more people will suffer breathing disorders, leading to an increased demand for methods to prevent and treat these diseases. To properly address this problem, it is necessary to gain a more complete understanding of the mechanics of respiration. This research constitutes a further step toward this goal by focusing on the coupled solid/liquid micromechanics of an idealized piece of lung tissue.

Gas exchange in mammalian lungs is efficient because 90% of lung volume is partitioned into a labyrinth of small, systematically connected air spaces termed alveoli. Because these air spaces are (at least partially) lined with a thin liquid film, the lung contains an extensive and a highly curved liquid-gas interface. Surface tension forces acting at this interface play a central role in respiratory mechanics, and it is of fundamental as well as practical interest to establish the mechanisms by which surface tension moderates the distribution of the liquid lining. Further research on the fluid dynamics of the alveolar liquid lining is needed to enable a complete understanding of the mechanical force balance, surfactant distribution and particulate transport within the lung parenchyma.

Anatomical studies have shown that the liquid lining accumulates in pools in the corners of polyhedral alveoli. During respiration, the alveolar walls (or septa) are subjected to a periodic strain, and liquid is drawn into and out of these pools by the wall movement. The objective of this research is to investigate how surface tension forces compete with the...
viscous stresses associated with substrate stretching to control the thin film distribution in the vicinity of an alveolar corner, where septal planes meet. For this purpose, a mathematical model is proposed that couples thin-film fluid dynamics to a stretching substrate; this model extends prior, related investigations by accounting for the corner geometry through a localized (regularized) substrate curvature term.

Key model parameters include the liquid lining volume and the substrate stretching frequency and amplitude. Numerical simulations of this model (a highly nonlinear partial differential equation) are used to characterize the dependence of the film distribution on these system parameters, while asymptotic analysis is used to gain insight into the dominant physical mechanisms. The simulations reveal that the film distribution exhibits qualitatively different behavior with variations in the amplitude and frequency of stretching. At low stretching frequency, new small scale regions are found that control the net fluid flux during stretching. At high frequency, large-amplitude pressure fluctuations are observed near the corner, which may affect capillary blood flow and alveolar stability. At $O(1)$ frequencies, a capillary wave propagates from the corner to the nearest contact point, where it is largely reflected. The analysis developed here provides insight into the physics underlying the bifurcations evident in the computational results.
CHAPTER 1

INTRODUCTION

A brief synopsis of the physical motivation for this research investigation is given, including relevant background information and a short literature review.

1.1 Alveolar Form and Function

The respiratory system is composed of the mouth, larynx, trachea, bronchi and bronchioles, which terminate in alveoli (see Figure 1-1). Since the majority of pulmonary gas exchange occurs within the alveoli, it is important to understand alveolar mechanics during respiration.

As evident in scanning electron micrograph (SEM) images, alveoli are approximately polyhedral in cross section (see Figure 1-1 and 2-1). The thickness of alveolar septa ranges from 2 – 10 $\mu$m, while septal planes are about 100 $\mu$m in length. This tissue is highly deformable and wet by a layer of liquid containing pulmonary surfactants secreted by type I and type II cells located on the alveolar tissue. Their primary role is to control the concentration of surfactant. Pulmonary surfactants are composed of many kinds of proteins and polymers. Combined with the liquid lining on the substrate, surfactants alter the surface tension force acting at the liquid/air interface to enable a balance with other forces including tissue tension and capillary distending gas pressure acting in the lung parenchyma. In addition to influencing surface tension forces, the distribution and movement of the liquid lining controls the transport of surfactants, inhaled toxins, pathogens and other particulate matter so as to protect the lung.
Figure 1-1: Illustration of human pulmonary system (left) and alveolar shape as imaged by SEM (right).

For these reasons, it is of interest to understand the fundamental mechanisms by which substrate geometry, substrate elasticity and (surfactant-regulated) surface tension control the distribution of the alveolar liquid lining. As a first step toward this goal, this thesis focuses on the competition between capillary pressure variations and substrate stretching, assuming constant surface tension and viscosity, and ignores the new thermodynamic phase formed by surfactants in the liquid lining.
1.2 Literature Review

Biomechanics research on the lung began in the 1960s (e.g. [1], [3]). References [1], [2] and [3] are examples in which classical mechanical theory was applied to lung research. As more advanced technologies were developed, many physiologists (e.g. [4]) collaborated with engineers to look into the small-scale mechanics of the lung. By the 1980s, significant experimental data was accumulated to give a systematic picture of the whole lung. For example, researchers categorized the parts of the lung parenchyma and understood each part’s functional morphology. Moreover, research on the tissue components in the lung and the micromechanics of the acinus and alveolar walls were also investigated (e.g. [4], [5]).

Pulmonary mechanics research can be divided into groups interested in the nose, bronchi and small airways. Most respiratory diseases occurs in bronchioles and alveoli, so research in these areas is intensive. Meanwhile, engineers have become interested in developing lung imaging technology; this work continues to serve as a useful guid for theoretical investigations (e.g. [6], [7] and [8]).

Even regarding alveolar research, some scientists have analyzed lung tissue structure [9] while others have focused on surfactants [10][11] and fluid transport. References [12], [13] are written by two authorities in this field. They summarize the basic engineering approach to pulmonary fluid dynamics research including the mathematical methods commonly used.

Several papers have been published dealing with the liquid lining distribution. Although reference [14] doesn’t treat pulmonary fluid directly, it describes a fluid distribution that may exist in the absence of alveolar wall stretching. Reference [15] focuses on the liquid lining distribution near an interior corner but in the absence of substrate stretching. Both [16] and [17] treat Marangoni flow on a flat, periodically-stretched substrate; in this case, surface-tension effects are dominated by surfactants, and capillary pressures are assumed negligible. Reference [18] includes both Marangoni and capillary stresses and substrate stretching, but their model does not incorporate a large, spatially-localized curvature near the junction of septal planes, which may be one of most important factors driving the redistribution of the liquid lining. The analysis given in [18] also assumes a larger liquid
volume than that treated here. The unique aspect of this thesis is its focus on the influence of substrate stretching on the liquid lining distribution near an alveolar corner. The focus on stretching is motivated by the objective of understanding the thin-film fluid dynamics during respiration, when the alveolar wall is (presumably) lengthened periodically. This thesis describes the fluid readjustment under various stretching frequencies and amplitudes.
CHAPTER 2

PROBLEM FORMULATION

In this chapter, a conceptual model is developed which forms the basis of the investigation. After invoking certain assumptions, the equation governing the evolution of the liquid lining during stretching is derived. The physical scales used in the lubrication approximation employed here are identified, as are the resulting non-dimensional parameters. Finally, an effective boundary condition near the alveolar substrate corner is derived for use in the theoretical analysis described in the following chapters.

2.1 Conceptual Model

As stated above, the objective of this research is to investigate the influence of the alveolar corner geometry and substrate stretching on the distribution of the thin liquid lining. The three-dimensional, fully-coupled elastic/fluid-dynamic problem in realistic, irregular alveolar geometries is exceedingly complex. Thus, a simplified conceptual model is sought that retains some of the essential physical features of the full problem. These features include: (1) a two-dimensional, regular hexagonal substrate geometry, as an idealization of the polyhedral cross-sectional shapes of actual alveoli (see Figures 2-1 and 2-2); (2) a prescribed, sinusoidally-varying substrate length, as an approximation to the periodic straining of alveolar septa during respiration; and (3) a small liquid lining volume, leading to a corner puddle with an effective contact point along the substrate. Furthermore, as shown in the right-hand schematic in Figure 2-2, only a subsection of the full hexagonal geometry is investigated, since symmetric thin-film distributions are assumed.
Figure 2-1: High resolution image of acinus showing alveoli in cross-section. Note alveolar corners formed by the junction of three septal planes.

Figure 2-2: Idealized two-dimensional alveolar geometry (left). Thin-film geometry investigated in this study (right).
Clinical data indicates that the liquid lining height $O(0.1 \, \mu m)$ is much smaller than the substrate length $O(100 \, \mu m)$. Additionally, pulmonary film flow is a low Reynolds-number phenomenon that can be adequately modeled as creeping flow with a no-slip boundary condition along the substrate. Therefore, lubrication theory [13] can be applied to build a mathematical model.

2.2 Thin Films on Curved Substrates

2.2.1 Lubrication equations

The motion of a two-dimensional film on a curved substrate is governed by the incompressibility constraint and the Navier-Stokes equations:

$$\nabla \cdot \mathbf{u}^* = 0, \quad (2.1)$$

$$\rho \frac{D\mathbf{u}^*}{Dt^*} = \nabla \cdot \mathbf{T}, \quad (2.2)$$

$$\mathbf{T} = -p^* \mathbf{I} + \mu \left( \nabla \mathbf{u}^* + \nabla \mathbf{u}^*^T \right), \quad (2.3)$$

where $\mathbf{u}^*$ is the film velocity, $\rho$ the film density, $\mu$ the film viscosity, $p^*$ the film pressure, and $t^*$ time. Throughout, asterisks are used to denote dimensional variables.

These equations are augmented by the following boundary conditions. Along the substrate, the no-slip and no-penetration conditions are enforced:

$$\mathbf{u}^*(s^*, n^* = 0, t^*) = \mathbf{e}_s, \quad (2.4)$$

where $s^*$ is an arc-length coordinate measured along the substrate from the corner, $n^*$ is a coordinate measured normal to the substrate and directed into the liquid film, $L^*(t^*)$ is the (dimensional) instantaneous length of the substrate, and $\mathbf{e}_s$ and $\mathbf{e}_n$ are unit vectors in the $s^*$ and $n^*$ directions, respectively.

Along the air-liquid interface, i.e. along $n^* = h^*(s^*, t^*)$, where $h^*(s^*, t^*)$ is the film thickness (measured normal to the substrate), kinematic and dynamic conditions are imposed.
The former requires the interface to remain a material surface for all time, implying

\[
\frac{Dh^*}{Dt^*} = 0, \tag{2.5}
\]

where \(D/Dt^*\) is the usual material derivative. The dynamic constraints include the zero tangential-stress condition and the Young–Laplace equation for normal stress, which can be compactly written as

\[
T \cdot n + \sigma k^* n = 0. \tag{2.6}
\]

\(\sigma\) is the air-liquid surface tension, assumed constant in this analysis, \(n\) is the unit normal vector to the interface directed into the air, and \(k^* = \nabla \cdot n\).

Finally, at the lateral boundaries, \(s^* = 0\) and \(s^* = L^*\) (i.e. the corner location and the midpoint between adjacent corners, respectively), symmetry requires a zero slope condition (\(\partial h^*/\partial s^* = 0\)). In addition, a zero mass-flux constraint at both lateral boundaries is imposed.

Distances in the \(s^*\) direction can be scaled with a typical substrate length, \(L_0\), while distances in the \(n^*\) direction are scaled by a typical film thickness, \(H_0\); the ratio of these length scales is given by \(\epsilon \equiv H_0/L_0\). Introducing the capillary velocity scale, \(U \equiv \epsilon^3 \sigma/\mu\), then a Reynolds number can also be defined,

\[
Re \equiv \frac{\rho U H_0}{\mu} = \epsilon^4 \frac{\rho \sigma L_0}{\mu^2}. \tag{2.7}
\]

Non-dimensionalizing as follows:

\[
(s, \epsilon n, \epsilon h, L) \equiv \frac{(s^*, n^*, h^*, L^*)}{L_0}, \tag{2.8}
\]

\[
t \equiv \frac{Ut^*}{L_0}, \tag{2.9}
\]

\[(u, \epsilon v) \equiv \frac{(u^*, v^*)}{U}, \tag{2.10}
\]

\[p \equiv \frac{L_0 p^*}{\epsilon \sigma}, \tag{2.11}
\]

\[k \equiv \frac{L_0 k^*}{\epsilon}. \tag{2.12}
\]

Finally, the dimensional substrate curvature, \(\kappa^*\), is scaled with a typical radius of curvature of the substrate, \(a\), i.e. \(\kappa = a\kappa^*\).
Assuming $\epsilon << 1$ and $\epsilon^2 Re << 1$, the non-dimensional equations and boundary conditions reduce to the lubrication equations

\[
\Sigma_t + q_s = 0,
\]

\[
\Sigma = h \left[ 1 - \left( \frac{\epsilon L_0}{a} \right) \frac{h\kappa}{2} \right],
\]

\[
q = -\frac{1}{3} h^2 p_s + \frac{s}{L} \dot{h} + O \left( \epsilon^2, \epsilon^2 Re, \epsilon \frac{L_0}{a} \right),
\]

\[
p_n = O(\epsilon^2, \epsilon^2 Re, \epsilon \frac{L_0}{a}),
\]

and

\[
p = -k + O \left( \epsilon^2, \epsilon^2 Re, \epsilon \frac{L_0}{a} \right),
\]

\[
h_s(0, t) = h_s(L, t) = 0,
\]

\[
k_s(0, t) = k_s(L, t) = 0,
\]

where subscript notation has been used to denote partial differentiation. The non-dimensional curvature of the air-liquid interface can be expressed in terms of $h$ and $\kappa$:

\[
k = h_{ss} \left[ 1 - \left( \frac{\epsilon L_0}{a} \right) h\kappa \right] - h_s \left[ 1 - \left( \frac{\epsilon L_0}{a} \right) h\kappa \right]_s
\]

\[
\left\{ \epsilon^2 h^2_s + \left[ 1 - \left( \frac{\epsilon L_0}{a} \right) h\kappa \right]^2 \right\}^{\frac{3}{2}}
\]

\[
+ \frac{\left( \frac{L_0}{ca} \right) \kappa}{\left\{ \epsilon^2 h^2_s + \left[ 1 - \left( \frac{\epsilon L_0}{a} \right) h\kappa \right]^2 \right\}^{\frac{3}{2}}}.
\]

The lubrication equations are formally valid for thin films having small interfacial curvature everywhere. Indeed, in the limit of uniformly thin films and small substrate curvature, such that $L_0/a$ is $O(\epsilon)$, the interfacial curvature can be approximated as

\[
k = h_{ss} + \kappa + O(\epsilon).
\]

In the absence of stretching, the lubrication equations then reduce to

\[
h_t + \left[ \frac{1}{3} h^3 (h_{ss} + \kappa) \right]_s = 0,
\]

in agreement with the result of [21]. As Rosenweig and Jensen [22] have argued, the “geometrically nonlinear” lubrication model— in which the complete expression for the interfacial
Curvature is retained—may describe the long-time behavior of thin films draining into puddles which have finite interfacial curvature. As long as gradients of interfacial curvature are small in the puddle region, the pressure is nearly uniform and, thus, accurately predicted by the exact Young–Laplace constraint. Furthermore, the use of the full expression for $\Sigma$ ensures that volume conservation is satisfied, this being effected in reality by small, but fully two-dimensional pressure variations.

2.2.2 The corner singularity

A sharp corner constitutes a discontinuity in substrate curvature and, thus, must be treated carefully. If $\alpha$ denotes the half-angle of the (interior) corner, and $\beta \equiv \pi/2 - \alpha$ is defined to be the angle between the $s$- and $x$-axes, the corner curvature is given by

$$\kappa(s) = 2\beta \delta(s),$$

(2.23)

where $\delta(s)$ is the Dirac delta function. Although the actual shape of the air-liquid interface is smooth, the lubrication equations “feel” this geometric singularity when a fixed non-zero slope condition is imposed at the corner, causing a singular volume flux very near to the corner. This behavior can be understood by considering a smooth approximation to the corner curvature, e.g.

$$\kappa^*(s^*) = \frac{\beta e^{-\left(\frac{2s^*}{a}\right)^2}}{a\sqrt{\pi}},$$

(2.24)

which upon non-dimensionalization becomes

$$\kappa(s) = \frac{\beta e^{-\left(\frac{s}{d}\right)^2}}{\sqrt{\pi}}.$$  

(2.25)

In (2.25), $d \equiv a/L_0$, the non-dimensional characteristic substrate curvature. Note that the sharp corner scenario is recovered in the limit as $d \to 0$.

A very shallow interior corner is temporarily considered, corresponding to the limit in which $\beta \to 0$. Specifically, $\beta = O(\epsilon) = O(d)$. In this case, the scalings previously introduced accurately represent the film thickness and slope close to the corner (since the film is thin there); thus, the non-dimensional quantities $h$ and $h_s$ are order unity in that region. The
pressure is estimated (i) within and (ii) outside the region of strong substrate curvature, i.e. for (i) \( s = O(d) \) and for (ii) \( s >> O(d) \), respectively. In region (i), noting that

\[
\frac{e}{d} h\kappa = O\left(\frac{\beta}{d}\right) = O(d),
\]

(2.26)

\[
\kappa_s = O\left(\frac{\beta}{d}\right),
\]

(2.27)

\[
\frac{e}{d} h\kappa_s = O(1),
\]

(2.28)

(2.20) reduces to

\[
k = \frac{\kappa}{\epsilon d} + h_{ss} + \frac{e}{d} h_s(h\kappa)_s + O(d) = O\left(\frac{1}{d}\right).
\]

(2.29)

Thus, from (2.17), the pressure in region (i) is also \( O(d^{-1}) \). In region (ii), however, \( \kappa \approx 0 \), and \( k \approx h_{ss} \), so the pressure is order unity. This mismatch in pressure, which occurs over a small distance \( d \), generates very large volume fluxes near \( s = 0 \).

### 2.3 A Regularized Model Equation

Guided by the considerations of the previous section, it is reasonable to consider the dynamics of a thin film on a smoothed alveolar corner in the small-\( \beta \) limit. The substrate curvature, \( \kappa \), is given by (2.25). Throughout, \( \beta = O(\epsilon) = O(d) \), and \( \Delta \equiv \beta/\epsilon \) is an \( O(1) \) parameter.

Even in the small-\( \beta \) limit, the geometrically nonlinear lubrication model cannot be simplified readily when \( d \) is also small. In particular, care must be taken when expanding the \( k_{ss} \)-term to insure that all relevant terms of a given order are retained. Rather than attempting to develop a rational model in this limit, it is appropriate instead to propose an \textit{ad hoc} model motivated by the form of the lubrication equations. Based on experience with other thin film models, it is anticipated that the flow structures exhibited by the \textit{ad hoc} model away from corner will be robust.

The model equation is based on retaining only the leading linear contributions to the interfacial curvature and density (based on the scalings given in the previous section);
namely,
\[ k = h_{ss} + \frac{\kappa}{cd} + \frac{\epsilon}{d} h_s (h\kappa)_s + O(\beta), \]  \hfill (2.30)
\[ \Sigma = h + O(\beta). \]  \hfill (2.31)

Furthermore, neglecting the third term on the right in (2.30) and, since \( \beta \to 0 \), replacing the arc-length coordinate \( s \) with \( x \), thereafter, the model equation is
\[ h_t + \left\{ \frac{h^3}{3} \left[ h_{xx} + \frac{\Delta e^{-\left(\frac{x^2}{\alpha}\right)^2}}{d\sqrt{\pi}} \right] \right\}_x + \left( \frac{L}{L_t} x h \right)_x = 0. \]  \hfill (2.32)

These equations are supplemented by the following symmetry and no-flux boundary conditions:
\[ h_x(0, t) = h_x(L, t) = 0, \]
\[ h_{xxx}(0, t) = h_{xxx}(L, t) = 0. \]  \hfill (2.33)

### 2.4 Effective Corner Boundary Condition

As described previously, a Gaussian substrate curvature term localized near the corner is included in the model thin film equation (2.32). This term is used to smooth the pressure profile, i.e. to eliminate the pressure singularity near the origin, which is crucial for obtaining reliable numerical results. For the theoretical analysis, however, it is more convenient to impose a non-zero slope condition at the origin and to remove the substrate curvature term from (2.32). The equivalence of these two formulations as \( d \to 0 \) is demonstrated below, where an effective slope boundary condition is derived from (2.32) and (2.33).

In order to investigate the fluid behavior near \( x = 0 \), it is convenient to rescale \( x \): for \( x = O(d) \), where \( d \ll 1 \) controls the width of Gaussian substrate curvature,
\[ x = d\bar{x}, h(x, t) = \eta(\bar{x}, t), \frac{\partial}{\partial x} = \frac{1}{d} \frac{\partial}{\partial \bar{x}}. \]  \hfill (2.34)

Substituting into (2.32):
\[ d^4 \eta_t + \frac{\eta^3}{3} (\eta_{xx} + \frac{\Delta de^{-\left(\frac{\bar{x}^2}{\alpha}\right)^2}}{\sqrt{\pi}})_{\bar{x}} + d^4 \frac{L_t}{L} (\bar{x} \eta)_{\bar{x}} = 0. \]  \hfill (2.35)
Figure 2-3: Conceptual model used in this research.

Expanding the inner solution:

\[ \eta(x, t) = \eta_0(x, t) + \delta \eta_1(x, t) + \cdots, \tag{2.36} \]

and substituting into (2.35) yields the leading order \((O(1))\) equation:

\[ \left( \frac{\eta_0^3}{3 \eta_0^{xx}} \right)_x = 0. \tag{2.37} \]

Integrating (2.37) and using the zero-flux boundary condition \((h_{xxx} = 0)\) at \(x = 0\) yields

\[ \frac{\eta_0^3}{3 \eta_0^{xxx}} = 0. \tag{2.38} \]

Thus,

\[ \eta_0(x, t) = \frac{1}{2} C_1 x^2 + C_2 x + C_3, \tag{2.39} \]

or, in terms of the original \(x\) coordinate,

\[ \eta_0 = \frac{1}{2} C_1 \frac{x^2}{d^2} + C_2 \frac{x}{d} + C_3. \tag{2.40} \]

For matching with the outer solution, \(C_1 = C_2 = 0\) in (2.40).
At $O(d)$,
\[
\left[ \frac{\eta_0^3}{3} (\eta_{1xx} + \frac{\Delta e^{-\frac{y^2}{4}}}{\sqrt{\pi}}) \right]_x + \left[ \eta_0^2 \eta_1 \eta_{0xxx} \right]_x = 0. \tag{2.41}
\]
However, considering the solution for $\eta_0$, the second term in (2.41) is zero. Again using the no-flux condition, (2.41) can be simplified to
\[
\eta_{1xx} + \frac{\Delta e^{-\frac{y^2}{4}}}{\sqrt{\pi}} = C_4, \tag{2.42}
\]
where $C_4$ is a constant. Integrating (2.42) yields:
\[
\eta_{1x} = C_4 x - \Delta \frac{1}{\sqrt{\pi}} \int_0^x e^{-\frac{s^2}{4}} ds + C_5. \tag{2.43}
\]
Using the boundary condition $\eta_{1x}(0,t)=0$,
\[
\eta_{1x} = C_4 x - \Delta \text{erf}(\frac{x}{2}). \tag{2.44}
\]
Now, the Van Dyke Matching Rule requires:
\[
\lim_{d \to 0, x \text{ fixed}} \frac{\partial \eta}{\partial x} = \lim_{d \to 0, x \text{ fixed}} \frac{\partial \eta_1}{\partial x} = \lim_{x \to 0} \frac{\partial h}{\partial x}(x,t) = \frac{\partial h}{\partial x}(0^+, t). \tag{2.45}
\]
Substituting (2.44) into (2.45),
\[
\lim_{d \to 0, x \text{ fixed}} \frac{\partial \eta_1}{\partial x} = \lim_{d \to 0, x \text{ fixed}} (C_4 x - \Delta \text{erf}(\frac{x}{2})) = (-\Delta \text{erf}(\infty)) + \lim_{d \to 0, x \text{ fixed}} C_4 \frac{x}{d}. \tag{2.46}
\]
Clearly, to get a finite value $C_4 = 0$.

Therefore, the effective boundary condition near the corner is:
\[
\frac{\partial h}{\partial x}(0^+, t) = -\Delta \equiv -s, \tag{2.47}
\]
where $s = \Delta$ is an $O(1)$ slope parameter. This effective boundary condition will be used in the subsequent theoretical analysis (see Figure 2-3), i.e.
\[
h_t + \left( \frac{h^3}{3} h_{xxx} \right)_x + \left( \frac{L}{L_{xx}} x \right)_x = 0, \tag{2.48}
\]
\[
h_x(0^+, t) = -s, h_x(L, t) = 0, h_{xxx}(0, t) = 0, h_{xxx}(L, t) = 0, \tag{2.49}
\]
while equation (2.32) and (2.33) will be used for the numerical simulations.
Table 2.1: Liquid film material properties

<table>
<thead>
<tr>
<th>Liquid viscosity</th>
<th>Liquid density</th>
<th>Surface tension</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01 g/cm³</td>
<td>1.0 g/cm³</td>
<td>70 dyn/cm</td>
</tr>
</tbody>
</table>

2.5 Physical Scales

To interpret the results obtained by solving the governing equation numerically, it is necessary specify the physical scales used in the definition of the governing non-dimensional parameters. Moreover, the original motive for studying a thin film on a stretching substrate is to mimic alveolar movement during respiration. The alveolar substrate tissue will expand during inhalation while it will contract during exhalation, an effect that is modeled here by varying the substrate length periodically. Table 2-1 list the liquid film material properties used in this investigation.

In the derivation of the lubrication approximation, the capillary velocity scale is defined as the ratio of surface tension to viscosity, while the pressure scale is defined as the ratio of the product of the liquid height and surface tension over the square of alveolar substrate length. Recall that $\epsilon$ equals the ratio of the typical liquid height to the characteristic substrate length. The capillary number is defined by the ratio of the product of viscosity and stretching velocity over the surface tension. Finally, the time scale of normal respiration is roughly 5 seconds per cycle. Typical physical scales, non-dimensional parameter values, and the time scale characterizing surface-tension readjustments are listed in Table 2-2.
### Table 2.2: Non-dimensional parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capillary velocity scale $U = \frac{\varphi}{\epsilon \mu}$</td>
<td>70 μm/s</td>
</tr>
<tr>
<td>Liquid height $H_0$</td>
<td>1 μm</td>
</tr>
<tr>
<td>Substrate length $L_0$</td>
<td>100 μm</td>
</tr>
<tr>
<td>Non-dimensional $\epsilon = \frac{H_0}{L_0}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Non-dimensional $Ca = \frac{\mu l}{\sigma}$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Pressure scale $P_0 = \frac{\rho g}{\rho_0}$</td>
<td>$1N/m^2$</td>
</tr>
<tr>
<td>Normal respiration time scale $t_0$</td>
<td>5s</td>
</tr>
<tr>
<td>Capillary time scale $t_0 = \frac{L_0}{U}$</td>
<td>1s</td>
</tr>
</tbody>
</table>
CHAPTER 3

NUMERICAL METHOD AND THEORETICAL ANALYSIS OF THE THIN-FILM DISTRIBUTION ON A STATIONARY SUBSTRATE

In this chapter, the finite difference algorithm used to solve the fourth order partial differential equation governing the thin-film evolution is presented, and the quasi-steady liquid distribution that obtains in the absence of substrate stretching is determined using both analytical and numerical methods.

3.1 Finite Difference Algorithm

To numerically solve the governing equation with associated boundary conditions, a finite-differencing scheme is employed. Since the substrate length will change with time during stretching, it is convenient to first recast the governing equation and boundary conditions in substrate-based Lagrangian (rather than the usual Eulerian fluid) variables.

Re-expressing the Eulerian variables $x$ and $h$ in terms of the Lagrangian variables $\xi$ and $H$, where
Equation (2.32) becomes

\[ H(x,t) = h(x,t)L(t), \]  

\[ H_t + Q_x = 0, \]  

or explicitly,

\[ H, + 0. \]  

The corresponding boundary conditions become:

\[ H(0,t) = H(L,t) = 0, \]  

\[ H_{xxx}(0,t) = H_{xxx}(L,t) = 0. \]  

Equation (3.6) and boundary conditions (3.7) and (3.8) are discretized using second-order-accurate spatial differencing. For numerical stability, a staggered (but equi-spaced) grid is employed, with \( H \) and \( P \) computed on one set of nodes, and \( Q \) computed on a second set of grid points located half-way between the former set. The finite difference form of model equations are:

\[ P(i) = -\frac{H(i+1) - 2H(i) + H(i-1)}{4(\Delta \xi)^2L^3} - \frac{\Delta}{d\sqrt{\pi}}e^{-\left(\frac{L(i)\Delta \xi}{2}\right)^2} \]  

\[ Q(i) = -\frac{(H(i+1) + H(i))}{2} \frac{P(i+1) - P(i)}{2 \Delta \xi} - \frac{1}{3L^3} \]  

where \( \Delta \xi \) is half of the constant distance between two Lagrangian grid points. In other words it is the constant distance between the two staggered sets of nodes. In addition, the node representing both \( P(1) \) and \( H(1) \) is located at the origin, so the node representing \( Q(1) \) is \( \Delta \xi \) to the right of the origin.
Typically, 1000 grid points are used in the computations. A computer program was written in Matlab to solve the governing equation (3.3) and boundary conditions (3.7) and (3.8); implicit time integration is carried out using the built-in function ODE15s, which is a variable-order, backward-difference adaptive solver for stiff equations. (The required Jacobian matrix is computed by finite differences.)

Owing to the rapidly-varying nature of the substrate curvature near $\xi=0$, it is necessary to insure adequate resolution in that region. Thus, another code was written in which the 1000 grid points were not equi-spaced; instead, 500 grid points were included in the region $0 < \xi < 0.2$ while the other 500 grid points were located within the region $0.2 < \xi < 1$. The mapping function used to relate the original equally spaced grid and the new grid is:

$$\chi = \frac{(b + 1)\xi}{2(a + \xi)}$$

where

$$a = \frac{\bar{\xi}L}{L - 2\bar{\xi}}, \quad b = \frac{a}{\bar{\xi}}.$$  \hspace{1cm} (3.12)

Half of the grid points are located between $0 < \xi < \bar{\xi} = 0.2$, and the remaining half between $\bar{\xi} < \xi < 1$.

The above algorithm is based on using the ODE15s command in Matlab 7.0, which employs adaptive time stepping. To reduce the simulation time and to test the previous codes, a third code was developed to time-advance the model equation using a different, semi-implicit time-stepping scheme in which the current value of the variable $H$ is used while the future value of the pressure $P$ replaces the original $P$. The final set of future $H$ values are computed by solving a linear system of equations. All three codes produced quantitatively similar results for a range of parameter values.

### 3.2 Numerical Results for a Stationary Substrate

For purposes of comparison, it is necessary to understand the liquid distribution that is obtained on a stationary substrate; this quasi-steady liquid distribution is also needed to
initialize the computations that incorporate stretching. Based on the liquid lining volume, the numerical results can be divided into two groups: in one case, the volume $V$ is larger than a critical volume $V_c$ and in the other case, $V$ is smaller than $V_c$. The former case is a steady state while the latter attains a quasi-steady state liquid distribution.

3.2.1 $V > V_c$

Figure 3-1 shows the steady distribution that results when $V = 1, s = 1.1$ and $d = 0.05$. One thousand grid points are employed. The solutions plotted in Figure 3-1 are obtained after 1000 time units.

The picture at the top of Figure 3-1 indicates the liquid distribution is parabolic away from the small region of Gaussian curvature; the picture at the bottom of Figure 3-1 shows the pressure distribution is spatially uniform. Indeed, a parabolic film profile is an exact steady state solution to the thin film equation (2.48) with effective slope boundary condition (2.49).

3.2.2 $V < V_c$

Figure 3-2 shows the corresponding results for $V = 0.07$. Again, $s = 1.1, d = 0.05$, and 1000 grid points are employed.

Clearly, the film distribution shown at the top of Figure 3-2 is not purely parabolic; instead, there is a small scale region separating two parabolic regions. The corresponding pressure distribution shown at the bottom of Figure 3-2 also supports the conclusion that the pressure jumps between the parabolic regions. Thus, assuming this small region does not allow for direct interaction between the other large-scale regions, an analysis can be carried out separately in the three regions. The region near the substrate corner (or $x = 0$) is called the “Puddle” region. The small scale region with minimum liquid height and thickness in the middle of the two parabolic regions is defined as the “Drainage” region. The third region including the end of the substrate is termed the “Droplet” region.

To demonstrate that the corner region is adequately resolved in these simulations, Figure
Figure 3-1: \( h(x, t) \) (top) and \( p(x, t) \) (bottom) profiles without stretching when liquid volume \( V = 1 > V_c \); \( t = 1000 \), when solutions have reached steady state. \( s = 1.1, \ d = 0.05, \) 1000 grid points. \( h(x, 0) = 1. \)
Figure 3-2: $h(x, t)$ (top) and $p(x, t)$ (bottom) profiles without stretching when liquid volume $V = 0.07 < V_c$; $t = 1000$, when solutions have attained a quasi-steady distribution. $s = 1.1$, $d = 0.05$, 1000 grid points. $h(x, 0) = 0.07$. 

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Figure 3-3: Comparison of solutions computed on non-equi-spaced (solid curve) and equi-spaced (circles) grids for $V > V_c$, $s = 1.1$, $d = 0.05$, 1000 grid points. $h(x, 0) = 1$. Compare with Figure 3-1.
Figure 3-4: Comparison of solutions computed on non-equi-spaced (solid curve) and equi-spaced (circles) grids for $V < V_c$. $s = 1.1$, $d = 0.05$, 1000 grid points. $h(x,0) = 0.07$. Compare with Figure 3-2.
3-3 and Figure 3-4 show the same results as in Figure 3-1 and Figure 3-2, respectively, but computed on a non-equi-spaced grid. Half of the grid points lie between $\xi = 0$ and $\xi = 0.2$ while the remaining grid points lie along the rest of the substrate. Figure 3-3 shows the profiles obtained when $V = 1$ while Figure 3-4 shows the case when $V = 0.07$. Comparing Figures 3-1 and 3-2 with Figures 3-3 and 3-4, it is evident that 1000 equi-spaced grid points provide adequate resolution of the corner; hence, this scheme is used in the following chapters.

3.3 Theoretical Analysis

As mentioned above, there are three regions to be discussed when the liquid lining reaches a quasi-steady distribution: the Puddle, the Drainage Region and the Droplet. In the absence of substrate stretching, the governing thin film equation reduces to:

$$h_t + \left( \frac{h^3}{3} h_{xxx} \right)_x = 0, \quad (3.13)$$

with effective slope boundary condition $h_x(0^+, t) = -s$ and the given homogeneous boundary conditions.

The following sections will simplify this general equation based on the fluid behavior in the different regions.

3.3.1 Puddle

In this region, the height of the film is $O(1)$ and variations in $h$ occur over an $O(1)$ scale in $x$. Additionally, sufficient time has passed ($t >> 1$) that transients have been eliminated and the puddle adjusts quasi-statically to the instantaneous fluid volume in that region, i.e. $h_t$ is negligible.

Thus, in this region the governing equation becomes:

$$(h^3 h_{xxx})_x = 0. \quad (3.14)$$
At the corner, $h$ satisfies zero-flux and specified slope conditions:

$$h_x(0^+, t) = -s, \quad h_{xxx}(0, t) = 0.$$  \hspace{1cm} (3.15)

Near the far edge of the puddle, the film height exhibits a minimum that, at leading order in inverse time, is zero, i.e.

$$h(x_0, t) = 0, \quad h_x(x_0, t) = 0,$$ \hspace{1cm} (3.16)

where $x_0(t)$ is the $x$-location at which the film height is minimum.

The solution of the above equation and boundary conditions is:

$$h(x, t) = \frac{s}{2x_0} - sx + \frac{s}{2} x_0,$$ \hspace{1cm} (3.17)

so in the puddle, the free surface has a parabolic shape. $x_0$ is determined from volume conservation, given (3.17), once the droplet solution is known:

$$\int_0^1 h(x) dx = V.$$ \hspace{1cm} (3.18)

The critical volume mentioned above refers to the special case in which $x_0 = 1$. Using (3.17) and (3.18), it is easy to show that $V_c = \frac{s}{6}$. Here, $s = 1.1$, so $V_c = \frac{11}{6}$. When $V < V_c$, $x_0 < 1$.

### 3.3.2 Droplet

Within the droplet, the film also evolves quasi-steadily over an $O(1)$ length scale. Meanwhile, the numerical simulations reveal that $h = O(t^{-\frac{1}{4}})$ in the droplet. Rescaling such that $h = t^{-\frac{1}{4}} F$, the governing thin film equation becomes:

$$-\frac{1}{4} t^{-\frac{5}{4}} F + t^{-\frac{1}{4}} F_t + t^{-\frac{1}{4}} \left( F^3 F_{xxx} \right)_x = 0.$$ \hspace{1cm} (3.19)

Assuming $F_t = o(t^{-\frac{3}{4}})$ (which can be confirmed \textit{a posteriori}), then the above equation reduces to:

$$(F^3 F_{xxx})_x = 0,$$ \hspace{1cm} (3.20)
Figure 3-5: $h(x,1000)$ in the puddle region for $V = 0.07$, $s = 1.1$, $d = 0.05$, 1000 grid points.

$h(x,0) = 0.07$. 

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subject to

\[ F_x(1, t) = 0, \quad F_{xxx}(1, t) = 0, \quad (3.21) \]

and, near the drainage region,

\[ F(x_0, t) = 0. \quad (3.22) \]

Note that (3.22) is appropriate because, near the drainage region, the numerical simulations reveal \( h = O(t^{-\frac{1}{2}}) \), i.e. in the drainage region, \( F = O(t^{-\frac{1}{4}}) \). Since \( F \) is \( O(1) \) in the droplet, the value of \( F \) should approach zero near the drainage region.

Moreover, to solve (3.20), a fourth boundary condition is needed; this is obtained by matching the slope of the film between the droplet and drainage zone.

Finally, the analytical solution in this droplet is:

\[ h(x, t) = t^{-\frac{1}{4}}c_1\left(\frac{x^2}{2x_0 - x_0^2} + \frac{2x}{x_0^2 - 2x_0} + 1\right), \quad (3.23) \]

where \( c_1 \) will be determined via matching with the drainage zone. Thus, the free surface shape of the droplet is also parabolic. The numerical results suggest the curvature in the droplet is opposite in sign to that in the puddle; compare Figure 3-6 with Figure 3-5.

### 3.3.3 Drainage region

Fluid is slowly pumped from the droplet to the puddle, owing to the difference in capillary pressures between these regions, through a very short drainage region. The shape of the free surface in this region, as determined from the numerical solution, is shown in Figure 3-7.

Based on many numerical simulations, it is found that \( h \) is \( O(t^{-\frac{1}{2}}) \) and \( x - x_0 \) is \( O(t^{-1/4}) \) in the drainage zone. Thus, \( h \) and \( x \) are rescaled as follows:

\[ h = t^{-\frac{1}{2}}H(r, t), \quad x = x_0(t) + t^{-\frac{1}{4}}r, \quad (3.24) \]

where \( H \) and \( r \) are \( O(1) \) variables.

Substituting the new non-dimensional variables into the model equation (3.13) yields
Figure 3-6: $h(x, 1000)$ in the droplet region for $V = 0.07$, $s = 1.1$, $d = 0.05$, 1000 grid points. $h(x, 0) = 0.07$. 

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Figure 3-7: $h(x, 1000)$ in the drainage region for $V = 0.07$, $s = 1.1$, $d = 0.05$, 1000 grid points. $h(x, 0) = 0.07$. 

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\[-\frac{1}{2} t^{-\frac{3}{2}} H + t^{-\frac{1}{2}} H_t + \frac{1}{3t} (H^3 H_{rrr})_r = 0 \quad (3.25)\]

Assuming \( H_t = o(t^{-1/2}) \) for \( t \gg 1 \), the first two terms are negligible compared to the last term; thus, the governing equation in the drainage region becomes:

\[(H^3 H_{rrr})_r = 0. \quad (3.26)\]

This equation can be integrated once to obtain:

\[H^3 H_{rrr} = -q, \quad (3.27)\]

where \( q \) is a constant which is related to the volume flux through the drainage region. According to the previous definition,

\[Q = -\frac{1}{3} p_x h^3 = \frac{1}{3} \frac{1}{2} t^{-\frac{5}{2}} H^3 H_{rrr}. \quad (3.28)\]

So based on the definition of \( q \), the relationship between \( q \) and \( Q \) is:

\[Q = \frac{1}{3} t^{-\frac{5}{2}} q. \quad (3.29)\]

Since \( H \) and \( r \) are both \( O(1) \) variables, \( q \) should be a \( O(1) \) constant, i.e. the magnitude of the flux through the drainage zone will be \( O(t^{-\frac{3}{4}}) \).

The conditions at the boundaries of the drainage region can be obtained by asymptotic matching with the adjacent regions: as \( r \to -\infty \),

\[H \sim \frac{s}{2x_0} r^2; \quad (3.30)\]

and as \( r \to \infty \),

\[H \sim 2c_1(\frac{1}{x_0^2} - \frac{x_0}{2x_0}) r. \quad (3.31)\]

Introducing two parameters \( c \) and \( z \), where

\[c \equiv \frac{s}{x_0}, \quad z \equiv 2c_1 \frac{1}{x_0^2} - \frac{x_0}{2x_0}, \quad (3.32)\]
these matching conditions become, as $r \to -\infty$,

$$H \sim \frac{c}{2} r^2,$$

and as $r \to \infty$,

$$H \sim zr,$$  \hspace{1cm} (3.34)

To remove all parameters except one from this boundary value problem (BVP), new variables $y$ and $u$ are introduced, where

$$u \equiv -A \frac{c}{2z^2} r, \quad y \equiv A \frac{c}{2z^2} H, \quad A \equiv \frac{cq}{2z^3}. \hspace{1cm} (3.35)$$

Consequently,

$$y_{uuu} y^3 = 1,$$ \hspace{1cm} (3.36)

subject to

$$y \sim A u^2, \text{ as } u \to \infty,$$ \hspace{1cm} (3.37)

$$y \sim -u, \text{ as } u \to -\infty.$$ \hspace{1cm} (3.38)

The nonlinear ordinary differential BVP (3.36)-(3.38) was solved numerically using a boundary value problem solver (bvp4c) in Matlab. Figure 3-8 shows the results of this numerical computation. The value of $A$ is returned as 0.548.

### 3.3.4 Unknown parameters

To completely specify the analytical solutions in the three different regions, three unknown parameters $q$, $x_0$ and $c_1$ must be determined. Thus, three equations are needed to obtain a global $h(x,t)$ analytical solution. One equation is derived from the definition of $A$ in (3.35): see (3.39). A second equation is based on volume conservation; neglecting the small film volume in the drainage region yields (3.40). The final equation, (3.41), is obtained by equating the rate of volume change in the droplet to the flux through the drainage zone.
Figure 3-8: Theoretical prediction of liquid distribution in drainage region obtained by numerical solution of BVP (3.36)-(3.38).
\[ A = \frac{cq}{2x_0^5} = \frac{s q (x_0^2 - 2x_0)^5}{2x_0(2c_1)^5(1 - x_0)^5}. \]  
(3.39)

\[ \int_0^{x_0} h(x)dx + \int_{x_0}^1 h(x)dx = V. \]  
(3.40)

\[ \frac{dV_{\text{droplet}}}{dt} = \frac{d}{dt} \left( \int_{x_0}^1 h(x)dx \right) = q. \]  
(3.41)

Obviously, (3.39) relates \( q \) to \( x_0 \) and \( c_1 \), with \( A = 0.548 \). Equation (3.40) indicates a relationship between \( x_0 \) and \( c_1 \). Thus, based on (3.39) and (3.40), \( q \) and \( c_1 \) can be expressed by \( x_0 \). So the remaining task is to determine the value of \( x_0 \). In fact, (3.41) provides an ordinary differential equation for \( x_0 \) as a function of time. Thus, an initial value is needed. Recalling there is a net flux of fluid pumped from the droplet region to the puddle region continuously, and assuming this pumping lasts infinite time, all of the fluid in the droplet region should be transported to the puddle region. Therefore, given the total liquid volume and the analytical solution for \( h \) in the puddle, it is easy to determine the value of \( x_0 \) when the pumping time is infinite, where this value can be defined as \( x_{0\infty} \). Then the three unknown parameters can all be computed.

In practice, the final result shows \( x_0 \) changes with time very slowly. Thus, it is reasonable to assume \( x_0 \) is a constant. Therefore, with \( V = \frac{1}{30} \) and this constant \( x_0 \), these three parameters are: \( x_0 = 0.43, q = 0.054, c_1 = -0.39 \).

### 3.4 Comparison

There is another way to test the solution in the drainage region. On p.378 of [14], the same model equation and boundary conditions as those used to describe the drainage region are derived for a different problem. Thus, Figure 3-8 shown here should be identical to Figure 5 in [14]. As an illustration, at \( u = 7 \) both graphics show \( y \approx 50 \) and they also indicate \( y_{\text{min}} \approx 1 \) around \( u = 0 \). (There is good agreement between Figure 3-8 and Figure 5 in [14] at other points, too.) In subsequent chapters, this “drainage region” is also called the “Hammond region”, where the concept of “drainage” is obscure in some stretching circumstances.
3.5 Computational Parameters

Unless stated otherwise, the following parameters are used in the numerical simulations discussed in subsequent chapters: \( s = 1.1, \ d = 0.05 \) and \( V = 0.07 \). Also, a minimum of 1000 grid points is used in these simulations, and the quasi-steady distribution shown in Figure 3-2 (i.e. computed after \( t = 1000 \) time units starting from a uniform distribution) is used as the initial condition.
Chapter 4

Sample Numerical Results for a Periodically-Stretched Substrate

Physiological data suggests that the liquid film volume in healthy alveoli is less than the critical liquid volume, as defined here. Therefore, this thesis focuses on the influence of stretching when $V < V_c$. For a given $V$, the numerical simulations show qualitatively different fluid behavior in different parts of $A-\omega$ parameter space, where $L(t) = 1 + A \sin(\omega t)$; i.e. $A$ is the stretching amplitude and $\omega$ is the frequency. Although the substrate is strained symmetrically, the film distribution does not exhibit a symmetric response. In addition, the liquid lining distribution depends on the absolute time, not simply on the phase within a given cycle. The following sections will briefly discuss some of these numerical results.

4.1 A Fixed, Variable $\omega$

Figure 4-1 shows the film height and pressure distributions obtained from the numerical simulations when $V = 0.07$ and $A = 0.1$; $h(x, t)$ and $p(x, t)$ are plotted at a given $t$ for various stretching frequencies, including $\omega = 10$, $\omega = 1$, $\omega = 0$ and $\omega = 0.1$. Here, because the stretching time equals a certain integer multiple of the stretching period, Eulerian
variables are identical to Lagrangian variables: $h = H, p = P$ and $x = \xi$.

From Figure 4-1, it is evident that the film height is not overly sensitive to $\omega$; in contrast, the film pressure is very sensitive to the stretching frequency. In these plots, "time 1" refers to the initial time at which the fluid distribution is recorded during the simulation. Here, it stands for $t = 40\pi$, starting at $t = 0$ with the initial quasi-steady Hammond film profile.

Figure 4-1 indicates that, for a given stretching amplitude varying the stretching frequency will result in a modification to the pressure distribution along the substrate. Figure 4-2 shows another interesting phenomenon: the location and value of the minimum fluid height, $x_{min}(t)$ and $h_{min}(t)$, respectively, also depend on the stretching frequency. Based on the discussion given in the previous chapter, this point is very important for defining the width of the puddle and the drainage regions.

### 4.2 $\omega$ Fixed, Variable $A$

Similarly, with fixed $\omega = \frac{2\pi}{6\Omega},$ Figure 4-3 and Figure 4-4 also show that $h(x, t)$ and $p(x, t)$ change with both space and time under different stretching amplitudes: $A = 0.0001$ and $A = 0.1$. Obviously, it is reasonable to reach a similar conclusion that varying the stretching amplitude will introduce new physical mechanisms which govern fluid movement during stretching at fixed frequency. These results stimulate the research into the response of the liquid film as $A$ and $\omega$ are systematically varied.

### 4.3 Asymmetric Response During a Single Cycle

There is another interesting phenomenon, which is evident in Figure 4-5. Noting that the substrate stretching is simulated by setting $L = 1 + A\sin(\omega t)$, during one cycle, the liquid height and pressure distributions should be the same when, e.g., $t = \frac{\pi}{4\omega}$ and $\frac{3\pi}{4\omega}$ if the film responds to the substrate movement immediately. However, Figure 4-5 reveals that this is not the case.

These two graphs are plotted in Eulerian rather than Lagrangian variables and depict
Figure 4-1: $h(x, 3200)$ (top) and $p(x, 3200)$ (bottom) profiles for $A = 0.1$ and $\omega = 0.1, 0, 1, 10$. 

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Figure 4-2: $h_{min}$ (top) and $x_{min}$ (bottom) versus time for $A = 0.1$ and $\omega = 0.1, 0.1, 1, 10$. 

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Figure 4-3: $h(x, 20)$ (top) and $p(x, 20)$ (bottom) profiles for $\omega = \frac{2\pi}{0.1}$ and $A = 0.0001, 0.1$. 

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Figure 4-4: $h_{\text{min}}$ (top) and $x_{\text{min}}$ (bottom) versus time for $\omega = \frac{2\pi}{T}$ and $A = 0.0001, 0.1$. 

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the real fluid movement along the substrate. Here, in Figure 4-5, the "time 1", "time 2" and "time 9" in the legend refers to $t = 0$, $t = \frac{\pi}{4\omega}$ and $t = \frac{2\pi}{\omega}$. The time increment is $\frac{\pi}{4\omega}$. (note that $t = 0$ actually refers to $t = t_0$, where $t_0$ is some large, integer number of cycles.)

It is evident that, except at the beginning and end of the cycle, the film height distribution does not repeat. In other words, the substrate stretching is symmetric but the film response is not!

This phenomenon can be explained by analogy with the Bretherton problem [18][19], which will be illustrated in the next chapter.

4.4 Dependence of Film Distribution on Absolute Time

Figure 4-6 shows the distributions of $h(x, t)$ and $p(x, t)$ at the initial stretching time, after 100 cycles and after 1000 cycles. It is clear that $p(x, t)$ after 100 cycles differ from $p(x, t)$ after 1000 cycles. This indicates the liquid height and pressure distributions will also depend on the absolute time, not simply the relative phase during the cycle.

4.5 Summary

In this chapter, sample computational results have been used to demonstrate that substrate stretching introduces new physics into the film readjustment problem, and that the film distribution depends on both time and the stretching parameters $A$ and $\omega$ in a complex way. In subsequent chapters, different regions in $A-\omega$ parameter space are investigated (see Figure 4-7) to explore the film distribution during stretching.
Figure 4-5: $h(x, t)$ at various times during the 60th cycle. $A = 0.1$, $\omega = 10$. Note $V = 0.0333$. 

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Figure 4-6: $h(x,t)$ (top) and $p(x,t)$ (bottom) profiles at $t = 0, 100T$ and $1000T$, where $T = \frac{2\pi}{\omega}$. $A = 0.1$, $\omega = 1$. ($V = 0.07$.)
Figure 4-7: Parameter space investigated in this study.
CHAPTER 5

UNI-DIRECTIONAL EXTENSION

As a first step toward understanding the competition between surface tension and substrate stretching, the response of the liquid film to uni-directional, constant speed extension is investigated. This case provides useful clues to the dominant physics during extension at low frequencies. For this purpose, \( L = 1 + vt \) and \( t >> 1 \) in this chapter.

5.1 Numerical Results

Figure 5-1 shows the numerically-computed film height and pressure distributions in Lagrangian variables, while Figure 5-2 shows the corresponding Eulerian results, at two different times. The former figure reveals certain flow features, i.e. for \( \xi > 0.2 \), change little with time apart from a kinematic adjustment associated with stretching. Figure 5-2 shows that other flow features, i.e. for \( x < 1 \), change little in the laboratory frame for sufficiently large time. Thus, useful insights into the flow physics can be obtained by viewing the solution in both Lagrangian and Eulerian variables.

From Figure 5-2, one interesting phenomenon that can be observed is that there is a "kink point" that develops at a fixed Eulerian location, \( x \approx 0.5 \), where the pressure jumps sharply. This pressure boundary layer replaces that associated with the Hammond region. In other words, in uni-directional stretching, the pressure jump occurs at that fixed location, after sufficient time, independently of the length of the substrate.
Figure 5-1: Lagrangian film height (top) and pressure (bottom) distributions. Stretching speed \( v = \frac{\xi}{50} \).
Figure 5-2: Eulerian film height (top) and pressure (bottom) distributions. Stretching speed $v = \frac{\pi}{50}$.
Figure 5-1 also indicates that, a small distance beyond that kink point, there is little change with time in the liquid height and pressure distribution over the rest of the domain. This implies that the fluid lying beyond the kink point responds in a simple, kinematic fashion to substrate stretching. In addition, the free surface between the corner and the kink point remains parabolic. Therefore, it is reasonable to divide the whole domain into three parts based on this kink point: a Corner puddle, a Bretherton region (the small region near the kink point) and a Lagrangian stretching region, which includes the Hammond and droplet regions described previously. Clearly, new physical mechanisms are involved during uni-directional stretching, implying the theoretical analysis will differ from that of the no-stretching case.

5.2 Theoretical Analysis

Figure 5-3: Large-time, three-region asymptotic structure of film in uni-directional stretching scenario.
For large $t$, the film distribution can be divided into three regions. Figure 5-3 illustrates their locations.

### 5.2.1 Problem formulation

As in the analysis given in the previous chapter, a perturbation method can be applied to obtain analytical solutions in the separate regions.

For convenience, the governing thin film equation and boundary conditions are re-stated here:

\[
\begin{align*}
    h_t + \left( \frac{h^3}{3} h_{xxx} \right)_x + \frac{L}{L} (x h)_x &= 0, \quad (5.1) \\
    h_x(0^+, t) &= -s, \quad h_x(L, t) = 0, \quad (5.2) \\
    h_{xxx}(0, t) &= 0, \quad h_{xxx}(L, t) = 0, \quad (5.3)
\end{align*}
\]

where $L = 1 + vt$.

### 5.2.2 Corner puddle

According to Figure 5-1 and Figure 5-2, the height and substrate length in this region are $O(1)$. For large $t$, the puddle adjusts quasi-statically, so $h_t$ is negligible at leading order. Since $\frac{L}{t} \sim \frac{1}{t}$ for $t \gg 1$, the last term is also negligible. The second term, capturing the effect of surface tension, is the dominant factor in this region. Thus, at leading order in $t^{-1}$, the governing equation and corresponding boundary conditions in this region are:

\[
\begin{align*}
    \left( \frac{1}{3} h^3 h_{xxx} \right)_x &= 0, \quad (5.4) \\
    h_{xxx}(0, t) &= 0, \quad h_x(0^+, t) = -s, \quad h(x_0, t) = 0, \quad h_x(x_0, t) = 0, \quad (5.5)
\end{align*}
\]

where $x_0$ is the kink point, centered on the Bretherton region and fixed in the Eulerian frame.

The analytical solution to the above problem is
where $k$ is defined as $\frac{s}{x_0}$, i.e. the free surface shape in the puddle is parabolic and the pressure is uniform.

5.2.3 Bretherton problem

Before discussing the analytical solution of Bretherton region, it is helpful to first understand what the Bretherton problem is and its analogy with this uni-directional stretching problem.

![Figure 5-4: Bretherton problem.](image-url)
When a large air bubble passes through a liquid-filled pipe, its shape will have fore-aft asymmetry, and the height of the liquid film deposited between the bubble and the pipe wall is determined by the moving bubble’s speed. Reference [19] gives the equation governing the evolution of the thickness $w$ of the thin liquid film between the bubble and channel walls in a frame of reference in which the bubble is stationary:

$$w^3 w_{xxx} = 1 - w; \tag{5.7}$$

here, $x$ measures distance along the wall. Solutions of this thin film equation show that the bubble’s leading meniscus is smooth and rear meniscus has a wave-like appearance, in accord with experimental results; see Figure 5-4. This problem is referred to as the “Bretherton problem”.

In the uni-directional stretching problem, the “bubble” is the liquid-air interface near the kink point. Locally, substrate extension is analogous to wall movement with a constant speed in the Bretherton problem: the liquid-air interface near that point is fixed and analogous to the leading meniscus of a stationary bubble, as shown in the upper schematic of Figure 5-4. According to reference [19], the leading meniscus will be smooth and the film thickness depends on the local stretching speed. In contrast, the rear meniscus is wavy, with concomitant oscillations in the film pressure distribution. Although not investigated in this chapter, this scenario will be relevant during slow contraction of the substrate (see chapter 6).

### 5.2.4 Bretherton region

From Figure 5-2 and many other computational results (see also [19]), it is found that the length and height of this region scale as

$$x - x_0 = \eta t^{-\frac{1}{3}}, \quad h = t^{-\frac{2}{3}} H, \tag{5.8}$$

where $\eta, H$ are $O(1)$ variables. Substituting this rescaling into (5.1), that equation becomes:

$$-\frac{2}{3} t^{-\frac{5}{3}} H + t^{-\frac{1}{3}} H_t + t^{-\frac{1}{3}} \frac{1}{3} (H^3 H_{\eta\eta\eta})_{\eta} + \frac{vt}{1 + vt} [(x_0 + t^{-\frac{1}{3}} \eta) H]_{\eta} = 0. \tag{5.9}$$
For $t >> 1$, assuming $H_t = o(t^{-\frac{3}{2}})$, the above equation reduces to:

$$\frac{1}{3}(H^3 H_{\eta\eta})\eta + x_0 H_{\eta} = 0,$$

(5.10)

Applying Van Dyke's rule yields the following matching conditions:

$$\eta \to -\infty, \quad H(\eta,t) = \frac{1}{2}k\eta^2; \quad \eta \to +\infty, \quad H(\eta,t) = H_\infty; \quad (5.11)$$

where $H_\infty$ is a constant representing the film height as the Lagrangian stretching region is approached from the Bretherton region.

Rescaling the variables: $\tilde{H} = \frac{H}{H_\infty}, \chi = \frac{(3x_0)^{\frac{1}{3}}}{H_\infty} \eta$, Bretherton's equation is obtained:

$$\tilde{H}^3 \tilde{H}_{\chi\chi\chi} = 1 - \tilde{H}.$$  

(5.12)

The boundary conditions are:

$$\chi \to -\infty, \quad \tilde{H} = \frac{1}{2}k\chi^2; \quad \chi \to +\infty, \quad \tilde{H} \to 1.$$

(5.13)

This boundary value problem has a unique solution which grows quadratically as $\chi \to -\infty$: $\tilde{H} \sim \frac{1}{2}H_2\chi^2$, where $H_2 \approx 0.64304$. With the matching condition in (5.13) as $\chi \to -\infty$, this implies that $H_\infty = \frac{H_2(3x_0)^{\frac{1}{3}}}{k}$. Thus, the film thickness deposited downstream of the "leading meniscus":

$$h_\infty \equiv t^{-\frac{3}{2}}H_\infty = \frac{H_2^{\frac{2}{3}}}{k}(\frac{x_0}{t})^{\frac{2}{3}}$$

(5.14)

is proportional to the local substrate speed $(\frac{x_0}{t})L \approx \frac{x_0}{t}$ to the two-thirds power.

Figure 5-5 shows the shape of the free surface $\tilde{H}$ and the film pressure distribution $\Phi$ in the Bretherton region as determined from the solution of (5.12) and (5.13). Here, $\tilde{H}$ is defined above: in analogy to the usual definition of pressure in thin films, $\Phi \equiv -\tilde{H}_{\chi\chi}$. In terms of the previously-defined fluid pressure, $\Phi(\chi, t) = \frac{H_\infty}{(3x_0)^{\frac{1}{3}}} P(x, t)$.

From Figure 5-5, it is found the free surface shape is almost flat. (The many "1"s appearing along the $y$ axis indicate a very small variation of $\tilde{H}$ along the $x$ axis may exist.) Meanwhile, the jump in the pressure-like variable $\Phi$ in Figure 5-5 accords well with the full numerical simulations and attests to the relevance of the above analytical solution.
Figure 5-5: Theoretical prediction of liquid height (top) and pressure (bottom) profiles in the Bretherton region.
5.2.5 Lagrangian stretching region

From Figure 5-1, Figure 5-2 and many other computational results, it is found that the length and height of this region scale as:

\[ x - x_0 = z, \quad h = t^{-\frac{5}{6}} g, \quad (5.15) \]

where \( g \) and \( z \) are \( O(1) \) variables. Substituting into (5.1) yields

\[ \left[ \left( -\frac{2}{3} t^{-\frac{5}{6}} g + t^{-\frac{5}{6}} g_t \right) + t^{-\frac{5}{6}} \left( \frac{2}{3} g_{zz} \right)_z \right] + \frac{v t^{-\frac{5}{6}}}{1 + vt} \left[ (x_0 + z) g \right]_z = 0. \quad (5.16) \]

Assuming \( g_t = O(t^{-1}) \), the leading order balance occurs at \( O(t^{-\frac{5}{6}}) \). Dropping the surface tension term, and returning to the original \( h(x, t) \) Eulerian variable yields

\[ h_t + \frac{1}{t}(x h)_x = 0. \quad (5.17) \]

The general solution of the above equation is \( h(x, t) = \frac{1}{t} g(\frac{x}{t}) \). For asymptotic matching as \( x \) approaches \( x_0 \),

\[ \frac{H}{t^{\frac{5}{6}}} = \frac{1}{t} g\left( \frac{x_0}{t} \right) = \frac{1}{t} \left[ c \left( \frac{x_0}{t} \right)^{-\frac{1}{3}} \right] \quad (5.18) \]

where \( c \) is a constant. The above equation determines \( g\left( \frac{x}{t} \right) \); thus, the analytical solution in this Lagrangian stretching region is:

\[ h(x, t) = \frac{H}{t^{\frac{5}{6}}} \left( \frac{x_0}{x} \right)^{\frac{1}{3}}, \quad (5.19) \]

i.e. \( h(x, t) \) varies as \( x^{-\frac{1}{3}} \) at a given time (see Figure 5-6). Again, this analytical solution agrees well with the results of the numerical simulations.

5.3 Physical Explanation

Unlike the Hammond problem that arose in the no-stretching case, the small scale region in this uni-directional extension scenario is the Bretherton region. It is the Bretherton region that controls the fluxes of fluid out of the corner puddle in this problem.
Figure 5-6: Comparison of theoretical (top) and numerical (bottom) film height $h(x,t)$ in the Lagrangian stretching region.
In the following chapters, the stretching amplitude and frequency parameter space will be explored to see what types of film distributions may be realized during oscillatory stretching.
Chapter 6

LOW FREQUENCY STRETCHING

As mentioned in Chapter 4, various imposed stretching conditions will yield new physical phenomena. In this chapter, small frequency stretching is considered because this limit has much in common with the uni-directional extension scenario, and yet also incorporates the time-periodic stretching that is the main focus of this research. Thus, it is a natural starting point from which to investigate the effect of oscillatory stretching. In $A-\omega$ parameter space, $\omega$ is fixed while $A$ is varied to see what new phenomena appear.

6.1 Physical Scales

Before proceeding to investigate low frequency stretching, it is first necessary to distinguish "low" and "high" frequency regimes.

The key parameter which distinguishes the different frequency regimes is $\Omega = \frac{\omega}{1/T_s}$, where, again, $\omega$ is the stretching frequency and $T_s$ is the time scale for the fluid to adjust to surface-tension-induced pressure variations. Given the non-dimensionalization employed in Chapter 2, $T_s = t_0 = O(1)$ in the corner puddle. However, from the analysis given in the proceeding chapters, it is evident that narrow regions along the substrate often control fluid fluxes. In these regions, the film thickness (i.e. height) is typically an order of magnitude smaller than in the puddle, implying that $T_s = O(10^3)$. Thus, $\Omega = 10^3 \omega$. Based on this observation, the low-frequency stretching regime may be expected to arise for $\omega \leq O(10^{-4})$, 

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while the high-frequency regime occurs for $\omega \geq O(1)$. In this chapter, $\omega$ is fixed at a value of $10^{-5}$. As mentioned previously, in this and subsequent chapters, the initial film distribution for the periodic-stretching simulations is obtained after 1000 time units of the no-stretching scenario, starting from a uniform (i.e. flat) fluid distribution at $t = 0$.

6.2 Small Amplitude Behavior

6.2.1 Numerical results

Figure 6-1 shows $h(x, t)$ obtained numerically for the following stretching parameters: $s=1.1$, $V=0.07$, $d=0.05$, $A=0.001$ and $\omega=10^{-5}$. The upper plot shows the profile obtained after stretching for 200 cycles, while the lower plot compares $h(x, t)$ after 20 and 200 cycles zooming in on the region $0.6 < x < 1$.

As evident from Figure 6-1, there are only three regions under this stretching scenario: the Puddle, the Hammond region and the Droplet, which is the same as that of no-stretching scenario. The reason that this low-frequency, small-amplitude stretching yields an identical fluid response as that without stretching can be found in the perturbation analysis: since both $\omega$ and $A$ are small, their product $\omega A$ is very small. Therefore, the stretching term in the thin film equation should not be expected to make any significant contribution to the dominant fluid dynamics because it is proportional to $\omega A$. Thus, the fluid distribution obtained in this periodic stretching case is nearly the same as in the no-stretching scenario.

6.3 Large Amplitude Behavior

6.3.1 Numerical results

Figure 6-2 shows the fluid distribution at moderate stretching amplitude ($A = 0.1$). Clearly, a new physical response is evident in this case. Figure 6-4 also supports this conclusion. At sufficiently large stretching amplitude, a wedge region and a Bretherton region appear. This new discovery motivates the following analytical investigation of this large amplitude stretching case.
Figure 6-1: \( h(x, t) \) for \( A = 0.001, \omega = 10^{-5} \). The lower plot shows the film structure near the contact point.
Figure 6-2: $h(x, t)$ for $A = 0.1, \omega = 10^{-5}$ after 40 and 60 cycles. Note the appearance of a wedge-like region near the contact point.
To guide the theoretical analysis, additional numerical results during one cycle are needed: film profiles are plotted at five different times (during cycle 60-61) in Figure 6-5 and Figure 6-6. In Figure 6-5, Lagrangian variables are employed, while in Figure 6-6, the results are plotted in Eulerian variables. In subsequent chapters, similar numerical results at these five phases of a single cycle will be presented. Figure 6-4 shows the five phases selected; in the legends of Figure 6-5 and Figure 6-6, these are referenced as '1', '2', '3', '4', '5', respectively.

Figure 6-3: Five phases chosen during one cycle to display snapshots of film height and pressure distributions.
Figure 6-4: Lagrangian film height (top) and pressure (bottom) distributions during 60th cycle. $A = 0.1$, $\omega = 10^{-5}$. 

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Figure 6-5: Eulerian film height (top) and pressure (bottom) distributions during 60th cycle. $A = 0.1, \omega = 10^{-5}$. 

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6.3.2 Theoretical analysis

Figure 6-6 is a schematic indicating five distinct regions, in which different physical effects are dominant. However, of those five regions, the three adjacent, interior (i.e. middle) regions, called the Bretherton, Wedge and Hammond regions, are the main interest of the following analysis because they control fluid fluxes during stretching. In fact, the puddle, Hammond and droplet solutions are discussed in detail in the previous chapters, and the numerical results suggest that these regions are not significantly modified by substrate stretching (apart from the obvious kinematic extension and contraction). Thus, the two new interior regions (Bretherton and wedge) are the main interest of this analysis.

To carry out the analysis, a method including multiple time and spatial scales is applied:

$$x - x_c = \omega^p \bar{x}(t, T), \quad h(x, t) = \omega^p H(\bar{x}, t, T), \quad T = \omega t,$$

where $x_c$ is the approximate location of the center of the Bretherton region. From the numerical results, $x_c$ is fixed if plotted in the Eulerian variable. Here, $t$ is the actual time, while $T$ is a slow time scale capturing evolution over many oscillations; $h$ and $x$ are unscaled.
variables, while $H$ and $\bar{x}$ are $O(1)$ variables.

The governing equation (2.32) becomes:

$$\omega^p (H_t + \omega H_T) + \frac{1}{3}(\omega^{4p-4s}H^3H_{xxx})_x + \frac{A\omega\cos T}{1 + Asin T}[(\omega^s\bar{x} + x_c)(\omega^{p-s}H)]_x = 0. \quad (6.2)$$

The different regions will have different dominant terms and correspondingly different behaviors.

### 6.3.3 Bretherton region

Based on the uni-directional extension results, it is reasonable to expect surface tension and stretching will be the dominant factors. In order to neglect the first term in (6.2), its $\omega$ exponent should be larger than that of the other two terms, while their $\omega$ exponents should be equal:

$$4(p - s) = 1 + p - s, \quad p + 1 > 4(p - s). \quad (6.3)$$

Then applying perturbation theory, (6.2) becomes:

$$O(1): H_t = 0; \quad (6.4)$$

$$O(\omega^{3p-4s}): \frac{1}{3}(H^3H_{xxx})_x + \frac{A\cos T}{1 + Asin T}(x_c H)_x = 0. \quad (6.5)$$

In addition, the puddle solution is already known from the previous analysis:

$$h(x) = \frac{s}{2x_c}(x - x_c)^2, \quad (6.6)$$

where $s=1.1$.

For matching with the puddle:

$$\lim_{x_{\text{fixed}}<x_c, \omega \rightarrow 0} h_{\text{Bretherton}} = c(x - x_c)^2, \quad (6.7)$$

where $c$ is an $O(1)$ constant. From (6.1), this requires that $H \sim c\bar{x}^2$ as $\bar{x} \rightarrow -\infty$ and, hence, that $p - 2s = 0$. Combining this requirement with (6.3) yields:
Also, from (6.3), \( p + 1 > \frac{4}{3} \) to neglect unsteadiness on the slow (\( T \)) scale; since \( p + 1 = \frac{5}{3} \), this condition is satisfied with these scalings. Thus,

\[
x - x_c = w^\frac{3}{5} \bar{x}, \quad h(x, t) = w^\frac{3}{5} H(\bar{x}, T).
\]

Integrating (6.5) yields

\[
\frac{1}{3} H^3 H_{xxx} + \frac{A \cos T}{1 + A \sin T} x_c H = \frac{A \cos T}{1 + A \sin T} x_c H_\infty, \tag{6.10}
\]

where \( H_\infty \) is the constant value of \( H \) when \( \bar{x} \to +\infty \). The other boundary condition is:

\[
\bar{x} \to -\infty, \quad H \sim \frac{1}{2} k \bar{x}^2 \tag{6.11}
\]

where \( k = \frac{x}{x_c} \). Rescaling the above equation by

\[
\bar{H} = \frac{H}{H_\infty}, \quad c_1(T) = \frac{A \cos T}{1 + A \sin T}, \quad \chi = \frac{(3c_1 x_c)^{\frac{4}{3}}}{H_\infty} \bar{x}, \tag{6.12}
\]

(6.10) becomes:

\[
\bar{H}^3 \bar{H}_{xxx} = 1 - \bar{H}. \tag{6.13}
\]

Note that the sign of \( c_1(T) \) depends on \( \cos T \). Therefore, during the extension phase, \( \chi \) has the same sign as \( \bar{x} \), and the boundary conditions are:

\[
\chi \to +\infty, \quad \bar{H} \sim 1; \quad \chi \to -\infty, \quad \bar{H} \sim \frac{1}{2} \frac{k H_\infty^2}{(3c_1 x_c)^{\frac{4}{3}}} \chi^2. \tag{6.14}
\]

During contraction, however, \( \chi \) and \( \bar{x} \) will have opposite signs, so the boundary conditions during this phase are reversed:

\[
\chi \to -\infty, \quad \bar{H} \sim 1; \quad \chi \to +\infty, \quad \bar{H} \sim \frac{1}{2} \frac{k H_\infty^2}{(3c_1 x_c)^{\frac{4}{3}}} \chi^2. \tag{6.15}
\]
Given the Bretherton problem (6.13), boundary conditions (6.14) and (6.15) immediately reveal an important asymmetry that is induced by periodic substrate stretching. From an asymptotic analysis of the solutions to (6.13) in the far-field region where $H \sim 1$ (either as $\chi \to \infty$ or $\chi \to -\infty$), or from the numerical solutions to this boundary value problem, it is evident that the film pressure increases monotonically as $\bar{x} \to \infty$ when $\cos T > 0$; in contrast, when $\cos T < 0$, the film pressure increases non-monotonically as $\bar{x} \to \infty$. These predictions explain the cause of the pressure variations observed in the full numerical simulations during a complete cycle of substrate stretching (see Figure 4-1 and 6-4, 6-5).

A code was written to solve BVP (6.13) with (6.14) or (6.15) using a built-in BVP solver (bvp4c) in Matlab. Reference [19] shows that, during extension, $H(\infty) = \frac{H_0(3x_c^0)}{x}$, but during contraction, the numerical results obtained here suggest $H(\infty) \approx 0$, implying little fluid passes through the Bretherton region during contraction.

The above results indicate an interesting physical phenomenon: during substrate extension, there will be a net flow coming through the Bretherton region, while during substrate contraction, there will be very little net flow coming back to the puddle region. This suggests that there will be some fluid deposited in the wedge, making its width grow with time.

### 6.3.4 Wedge region

In this region, the substrate length and height are still defined as:

$$x - x_c = \omega^s \bar{x}, \quad h(x, t) = \omega^p H(\bar{x}, t, T),$$

(6.16)

where $H$ and $\bar{x}$ are $O(1)$ height and length variables in this region; however, $s$ and $p$ differ from their values in the previous subsection.

The numerical simulations (see Figures 6-2 and 6-4, 6-5) and the results of the unidirectional extension scenario suggest that volume change and stretching will be the dominant factors in this region. For surface-tension effects to be negligible in (6.2),
\[ p + 1 = p - s + 1, \quad p + 1 < 4(p - s), \] (6.17)

implying \( s = 0 \). Since, the width of the wedge is (asymptotically) finite, unlike the wedge width in uni-directional extension, \( p = \frac{3}{2} \) for matching with the right end of the Bretherton region:

\[ h \sim \omega^{\frac{3}{2}} H_{\infty} \sim \omega^p H(\bar{x}, t, T), \] (6.18)

Therefore, the scalings in the wedge region are

\[ x - x_c = \bar{x}, \quad h = \omega^{\frac{3}{2}} H(\bar{x}, T), \] (6.19)

yielding the following leading-order equation for the film height:

\[ H_T + \frac{AcosT}{1 + AsinT} [(x_c + \bar{x})H]_x = 0. \] (6.20)

Defining \( Y = (x_c + \bar{x})H \), the above equation can be recast as:

\[ \frac{1 + AsinT}{AcosT} Y_T + (x_c + \bar{x})Y_{\bar{x}} = 0. \] (6.21)

This first order partial differential equation can be solved by the method of characteristics:

\[ \frac{d\bar{x}}{ds} = x_c + \bar{x}, \quad \frac{dT}{ds} = \frac{1 + AsinT}{AcosT}, \quad \frac{dY}{ds} = 0, \] (6.22)

with initial conditions: \( T(0) = 0, \bar{x}(0) = \bar{x}_0 \). \( \bar{x}_0 \) is a constant describing \( Y \)'s initial location along the characteristic line, and it is needed to determine the relationship of \( x \) and \( T \) with \( s \). Figure 6-8 shows the relationship between \( x \) and \( T \), i.e. the characteristic curves.

Solving the above equations,

\[ Y = f(\frac{x - Ax_c sinT}{1 + AsinT}) = f(\frac{x - x_c - Ax_c sinT}{1 + AsinT}) = f(\frac{x}{1 + AsinT} - x_c) = f(\frac{x}{1 + AsinT}). \] (6.23)

Figure 6-10 shows the solution for \( Y \) at various times during one cycle assuming the initial profile \( f(z) = (z - 0.6)^2 + 0.1 \).
Figure 6-7: Characteristic curves $T(x)$, where $x = x_c + \bar{x}$, for (6.21).
Figure 6-8: Wedge solution $Y(x, T)$ at various times during one cycle.
Transforming the variable $Y$ into the Eulerian variable $h$ gives:

$$h = \frac{\sigma^3}{x} f\left(\frac{x}{1 + A\sin(\omega t)}\right). \quad (6.24)$$

The above function indicates the wedge solution is a moving wave. However, unlike a free wave, the end of this wave is asymptotically pinned at the origin as the profile is stretched out with time. The velocity of this bound wave is

$$\frac{dx}{dt} = \frac{x \cos T}{1 + A \sin T},$$

which is the same as the local substrate stretching speed.

### 6.4 Discussion

A new pressure boundary layer centered in the Bretherton region is found in this low-frequency stretching scenario, for sufficiently large amplitudes. This is expected from the understanding of the uni-directional stretching problem. Because of the appearance of the Bretherton region, a non-monotonic pressure profile during contraction is expected, as observed in the numerical results. According to the analysis, a net fluid flux coming through the Bretherton region during extension is found, in agreement with the simulations, while almost no net flux through the Bretherton region is predicted nor observed during contraction. This may explain why the width of the wedge region appears to grow with time. In contrast to the uni-directional scenario, the kink point location ($x = 0.63$) in this case is much closer to the effective contact point. Finally, for sufficiently small $\omega$ and small $A$, the numerical results indicate a similar fluid behavior as for the Hammond problem. Thus, it is expected that a bifurcation in the solution structure exists for low frequency stretching as $A$ is increased.
CHAPTER 7

HIGH FREQUENCY STRETCHING

In this chapter, the fluid redistribution caused by high-frequency stretching is investigated. This parameter regime is of particular clinical interest because prematurely-born infants, suffering respiratory distress, are often mechanically ventilated using a high-frequency, small-amplitude protocol.

7.1 Numerical Results

Figure 7-1 and Figure 7-2 show the film height and pressure profiles for a stretching amplitude \( A = 0.1 \) and a stretching frequency \( \omega = 10^4 \) with \( d = 0.01 \) at five times during cycle 60-61 in Lagrangian and Eulerian variables, respectively. The instantaneous film height appears to differ little from the stationary substrate scenario; however, the film pressure exhibits large-amplitude fluctuations very close to the corner. Thus, the high frequency stretching appears to act as a screening mechanism, confining disturbances to the free surface to a localized region.

7.2 Theoretical Analysis

To investigate this screening phenomenon, a multiple time and spatial scale asymptotic method is again employed.
Figure 7-1: Lagrangian film height (top) and pressure (bottom) distributions during 60th cycle. $A = 0.1$, $\omega = 10^4$. Note $d = 0.01$. 

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Figure 7-2: Eulerian film height (top) and pressure (bottom) distributions during 60th cycle.

$A = 0.1$, $\omega = 10^4$. Note $d = 0.01$.  

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7.2.1 Outer solution

Away from the corner, the problem is most conveniently analyzed in Lagrangian variables:

\[ H_t + \frac{1}{3L^7}(H^3H_{\xi\xi\xi})_{\xi} = 0; \]

\[ H_\xi(0^+, t) = -sL(t)^2, \quad H_{\xi\xi}(0, t) = 0, \quad H_\xi(1, t) = 0, \quad H_{\xi\xi}(1, t) = 0. \]

The analysis can be further simplified by defining \( \tau \) as the solution to

\[ \frac{d\tau}{dt} = -\frac{1}{3L(t)^7}, \]  

yielding:

\[ H_\tau + (H^3H_{\xi\xi\xi})_{\xi} = 0; \]

\[ H_\xi(0^+, \tau) = -sL(\tau)^2, \quad H_{\xi\xi}(0, \tau) = 0, \quad H_\xi(1, \tau) = 0, \quad H_{\xi\xi}(1, \tau) = 0, \]  

where \( L(\tau) \equiv L(t) \). This problem can be analyzed using two time scales: \( T = \omega \tau \) and \( \tau \), i.e. \( H_\tau \rightarrow H_\tau + \omega H_T \). Note that \( T \) is a fast time scale. Also, note that, with this prescription, the substrate length \( L(t) = 1 + A\sin(\omega t) \) essentially varies on the fast \( (T) \) scale. To make this dependence explicit, introduce \( \hat{T} \equiv \omega t \), so that:

\[ L(t) \rightarrow L(\hat{T}) \equiv 1 + A\sin(\hat{T}) \equiv L(T). \]  

Equation (7.1) can then be recast as:

\[ \frac{dT}{d\hat{T}} = \frac{1}{3L(\hat{T})^7}. \]  

Furthermore, in the large-\( \omega \) limit, \( H \) can be expanded as

\[ H(\xi, \tau; \omega) = H_0(\xi, \tau, T) + \frac{1}{\omega}H_1(\xi, \tau, T) + \cdots. \]
Substituting into (7.2) yields:

\[(H_{0\tau} + \frac{1}{\omega} H_{1\tau}) + \omega[H_{0T} + \frac{1}{\omega} H_{1T}] + [(H_{0} + \frac{1}{\omega} H_{1})^{3}(H_{0} + \frac{1}{\omega} H_{1})_{\xi\xi}\xi + \cdots = 0. \quad (7.7)\]

The inhomogeneous boundary condition in (7.3) becomes

\[H_{\xi}(0^{+},\tau) = H_{0\xi}(0^{+},\tau,T) + \frac{1}{\omega} H_{1\xi}(0^{+},\tau,T) + \cdots = -sL(T)^{2}. \quad (7.8)\]

At \(O(\omega)\), (7.7) requires

\[H_{0\tau} = 0, \quad (7.9)\]

i.e. \(H_{0} = H_{0}(\xi,\tau)\). However, the leading-order slope boundary condition requires

\[H_{0\xi}(0^{+},\tau) = -sL(T)^{2}. \quad (7.10)\]

In other words, the leading order equation indicates \(H_{0}\) is independent of \(T\), while the leading-order boundary condition requires \(H_{0}\) to vary with \(T\). The only way to resolve this apparent contradiction is through the existence of a boundary layer near the origin which provides a \(T\)-dependent slope boundary condition at the origin, and a \(T\)-independent slope boundary condition at the far-field edge of the boundary layer. Thus, the analysis given here can only be used to derive the outer solution. A multi-scale time and space method is needed to obtain the inner (boundary layer) solution; this analysis is carried out in the next subsection.

To determine how \(H_{0}\) varies with \(\tau\) and \(\xi\), the \(O(1)\) terms in (7.7) are set to zero:

\[H_{0\tau} + H_{1T} + (H_{0}^{3}H_{0\xi\xi})_{\xi} = 0. \quad (7.11)\]

Averaging (denoted by \(<.>\)) the above equation over the fast \((T)\) time scale, the first and third terms remain unchanged, but the second term becomes

\[<H_{1T}> = \frac{H_{1}(T) - H_{1}(0)}{T}. \quad (7.12)\]

To insure \(H_{1}\) varies sub-linearly with \(T\) (i.e. to suppress secular growth),

\[H_{0\tau} + (H_{0}^{3}H_{0\xi\xi})_{\xi} = 0. \quad (7.13)\]
Thus, away from the corner boundary layer, and over very many stretching cycles, the liquid layer satisfies a thin-film equation that is formally identical to (7.2) but subject to a time-independent effective slope boundary condition near the corner. A quasi-steady Hammond profile in $(\xi, \tau)$ coordinates is, therefore, expected.

### 7.2.2 Inner solution

The effective slope boundary condition for the outer solution can only be determined by analyzing the inner region (or boundary layer). In this region, $h = O(1)$, but spatial derivatives are large. Introducing

$$\xi = \omega^{-b} \eta$$  \hspace{1cm} (7.14)

where $b > 0$ is a constant to be determined, derivatives transform as

$$\partial_\xi = \omega^b \partial_\eta.$$  \hspace{1cm} (7.15)

The film height is expanded as:

$$H(\xi, \tau, T) \equiv F(\eta, \tau, T) = F_0(\eta, \tau, T) + \omega^{-a} F_1(\eta, \tau, T) + \cdots,$$  \hspace{1cm} (7.16)

where $a$ is a second constant to be determined.

The inhomogeneous slope boundary condition can be written as:

$$\omega^b [F_{0\eta} + \omega^{-a} F_{1\eta}](0^+, \tau, T) = -sL(T)^2.$$  \hspace{1cm} (7.17)

To obtain a sensible boundary condition it is necessary to set $a = b$, then

$$F_{0\eta}(0^+, \tau, T) = 0, \quad F_{1\eta}(0^+, \tau, T) = -sL(T)^2.$$  \hspace{1cm} (7.18)

The corresponding governing equation in this region is:

$$(F_0 + (\frac{1}{\omega})^a F_1)_\tau + \omega(F_0 + (\frac{1}{\omega})^a F_1) + \omega^{4b} [(F_0 + (\frac{1}{\omega})^a F_1)^b (F_0 + (\frac{1}{\omega})^a F_1)_{\eta\eta}] + \cdots = 0.$$  \hspace{1cm} (7.19)

The exponent $b$ is determined by incorporating unsteadiness on the fast $(T)$ scale and surface tension effects at leading order. Since the dominant unsteady term in (7.19) is $O(\omega)$, $4b = 1$, implying $b = a = \frac{1}{4}$ to achieve the desired balance.
The leading order problem, arising at \( O(\omega) \), is:

\[
F_{0T} + (F_0^3 F_{0\eta\eta\eta})_\eta = 0, \quad (7.20)
\]

subject to homogeneous derivative boundary conditions. By taking the inner limit of the outer solution, the solution to (7.20) is \( F_0(\eta, \tau, T) = H_0(0^+, \tau) \), i.e. the leading order inner solution is spatially uniform and varies only on the slow (\( \tau \)) time scale.

At \( O(\omega^3) \),

\[
F_{1T} + F_0^3 F_{1\eta\eta\eta} = 0, \quad (7.21)
\]

subject to the inhomogeneous slope boundary condition: \( F_{1\eta}(0^+, \tau, T) = -sL(T)^2 \). Before proceeding to solve (7.21), it is necessary to find the relationship between \( \tau \) and \( t \) (or \( T \) and \( \hat{T} \)) and to determine the explicit functional form of \( L(T) \).

### 7.2.3 Relationship between \( \tau \) and \( t \)

There are two ways to find the relationship between \( \tau \) and \( t \). One is strictly analytical, but is applicable only for small stretching amplitudes. The other approach is valid for arbitrary stretching amplitudes, but is partly numerical.

**Semi-analytical method**

In general, based on the periodic properties of \( \frac{1}{3\ell^2} \), it is straightforward to transform this function into its Fourier transform representation. Then this new representation can be easily integrated and the final relationship between \( \tau \) and \( t \) can be determined.

For example, upon choosing \( A = 0.1 \) and using 1024 grid points per cycle (\( \ell \)), the Fast Fourier Transform of \( \frac{1}{3\ell^2} \) can be obtained using standard library software, e.g. "fft" in Matlab. Thereafter, by investigating the power spectrum of this Fourier transformed function, it is observed modes 1 and -1 have two large peaks, modes 2 and -2 have relatively smaller peaks, and the mean mode has the largest peak. Here, the small peaks whose
amplitude is above 1% of the large peak of modes 1 and -1 are retained. For $A = 0.1$, only modes 2 and -2 satisfy this criterion. Thus, in this case,

$$\frac{1}{3(1 + A\sin(\omega t))^2} \approx a_0 + a_1 e^{i\omega t} + a_{-1} e^{-i\omega t} + a_2 e^{i2\omega t} + a_{-2} e^{-i2\omega t},$$

(7.22)

where $a_0, a_1, a_{-1}, a_2, a_{-2}$ are the mean, mode 1, -1 and mode 2, -2 coefficients. To obtain the numerical values of these coefficients, the Fast Fourier Transform representation can be employed:

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} (\hat{x}_k e^{2\pi i kn}),$$

(7.23)

for some function $x_n$ and its transform $\hat{x}_k$. (Thus, the coefficients of modes, 1, -1 and modes 2, -2 can be obtained by the Fast Fourier Transform value at entries 2, 1024 and 3, 1023 of the row vector divided by the total number of grid points $N(1024)$.)

The relationship between $\tau$ and $t$ is:

$$\tau = \int_0^t (a_0 + a_1 e^{i\omega t} + a_{-1} e^{-i\omega t} + a_2 e^{i2\omega t} + a_{-2} e^{-i2\omega t}) dt,$$

(7.24)

which results

$$\tau = a_0 t + \frac{a_1 - a_{-1}}{i\omega} (\cos(\omega t) - 1) + \frac{a_2 + a_{-2}}{\omega} \sin(2\omega t).$$

(7.25)

If a different stretching amplitude $A$ is selected, the above Fast Fourier Transform method can also be applied. To accurately determine the relationship between $\tau$ and $t$, however, the values of the coefficients, and the number of modes that must be retained for a given accuracy, will in general depend on $A$. 

---

Table 7.1: Fast Fourier Transform coefficients

<table>
<thead>
<tr>
<th>$a_{-2}$</th>
<th>-0.02515776648365</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{-1}$</td>
<td>-0.12766397735731i</td>
</tr>
<tr>
<td>$a_0$</td>
<td>0.38272405422349</td>
</tr>
<tr>
<td>$a_1$</td>
<td>0.12766397735731i</td>
</tr>
<tr>
<td>$a_2$</td>
<td>-0.02515776648365</td>
</tr>
</tbody>
</table>
Small-amplitude analytical formula

For arbitrary $A$, $\tau(t)$ satisfies

$$\frac{d\tau}{dt} = \frac{1}{3(1 + A\sin(\omega t))^2}. \quad (7.26)$$

Assuming $A$ is small, the right-hand-side can be expanded in a Taylor series about $A = 0$; retaining $O(A^2)$ terms, this gives:

$$\frac{d\tau}{dt} = \frac{1}{3}(1 - 7A\sin(\omega t) + 28A^2(\sin(\omega t))^2). \quad (7.27)$$

Integrating (7.27), and imposing $\tau(0) = 0$, yields

$$\tau = \frac{1}{3}[t + \frac{7A}{\omega}(\cos(\omega t) - 1) + 14A^2t - \frac{7A^2}{\omega} \sin(2\omega t)]. \quad (7.28)$$

Recalling that $T = \omega\tau$ and $\tilde{T} = \omega t$, the above equation can be used to relate these fast time scales:

$$T = \frac{1}{3}[\tilde{T} + 7A(\cos(\tilde{T}) - 1) + 14A^2\tilde{T} - 7A^2\sin(2\tilde{T})]. \quad (7.29)$$

Thus, for very small $A$, $\tilde{T} = 3T$.

The slope boundary condition requires $L(T)^2 = L(\tilde{T})^2 = (1 + A\sin(\tilde{T}))^2$. In order to retain terms as small as $O(A^2)$ in the expression for $L(T)^2$, only terms as small as $O(A)$ need be kept in the $\sin(\tilde{T})$ expression. Thus, using the relationship between $T$ and $\tilde{T}$ derived above,

$$\sin(\tilde{T}) \approx \sin(3T - 7A\cos(3T) + 7A), \quad (7.30)$$

or to $O(A)$,

$$\sin(\tilde{T}) = \sin(3T)\cos(7A) - \frac{7A\cos(7A)}{2}\cos(6T) + \sin(7A)\cos(3T) + \frac{7A\sin(7A)}{2}\sin(6T) - \frac{7A\cos(7A)}{2}. $$

Substituting into $L(\tilde{T})^2$ yields a formula for $L(T)^2$ that is accurate to $O(A^2)$:
\[ L(T)^2 = (1 - 7A^2 \cos(7A) + \frac{A^2(\cos(7A))^2}{2}) - \left( \frac{A^2(\cos(7A))^2}{2} + 7A^2 \cos(7A) \right) \cos(6T) + 2A \cos(7A) \sin(3T) + 2A \sin(7A) \cos(3T) + 7A^2 \sin(7A) \sin(6T). \]

As an illustration, \( A = 0.1 \) is selected to test the accuracy of this approach. From (7.28),

\[ \tau = 0.380000t + \frac{0.233333}{\omega} (\cos(\omega t) - 1) - \frac{0.023333}{\omega} \sin(2\omega t). \] (7.31)

Comparing (7.31) with (7.24) discussed in the previous section, it is evident that the coefficients differ by a relative error of less than 10%. Therefore, this method is the same as the general method when \( A \) is small enough.

The expression for \( L(T)^2 \) is composed of 3 terms: the constant term is the slope of external solution (as proved subsequently), and one of the remaining terms involves \( \cos 3T \) and \( \sin 3T \), while the other involves \( \cos 6T \) and \( \sin 6T \).

The equation and boundary conditions for \( F_1 \) are linear, and, hence, can be expressed as the sum of three components, denoted \( F_{1a}, F_{1b} \) and \( F_{1c} \), discussed next.

**Component a \( (F_{1a}) \): mean contribution**

\[ F_{1a} + F_{1a}^3 F_{1a} = 0; \] (7.32)

\[ F_{1a}(0, \tau, \eta) = -s(1 - 7A^2 \cos(7A) + \frac{A^2(\cos(7A))^2}{2}) \equiv -s\Gamma, \quad F_{1a}(0, \tau, T) = 0. \] (7.33)

Since the boundary conditions are independent of time, the solution \( F_{1a} \) is steady and, for matching with the external solution, varies linearly with \( \eta \):

\[ F_{1a} = -(\Gamma)\eta. \] (7.34)

**Component b \( (F_{1b}) \): 3rd harmonic**

A solution is sought of the form \( F_{1b} = B(\eta, \tau) \sin(3T) + C(\eta, \tau) \cos(3T) \). Defining \( G = B + iC \), the equation and boundary conditions governing \( F_{1b} \) reduce to the following problem for \( G \):
\[
F_0^3 G_{\eta \eta \eta \eta} + 3iG = 0; 
\]

(7.35)

\[
G_{\eta}(0, \tau) = -2As \cos(7A) - i(2As \sin(7A)), \quad G_{\eta \eta \eta \eta}(0, \tau) = 0. 
\]

(7.36)

Thus, \( G \) satisfies a fourth-order ordinary differential equation. Although only two boundary conditions are explicitly stated here, matching with the external solution requires that \( G \) remain bounded as \( \eta \to \infty \); this suffices to determine the remaining two constants in the \( G \) solution. With \( G \) known, \( F_{1b} \) can be given by:

\[
F_{1b} = c_1 e^{-\frac{1}{F_0}(-3iF_0)^{\frac{1}{2}} x} + c_2 e^{-\frac{1}{F_0}(-3iF_0)^{\frac{1}{2}} x}, 
\]

(7.37)

where \( c_1 \) and \( c_2 \) are both constants. Their values are

\[
c_1 = \frac{2420189F_0}{14170000(-3iF_0)^{\frac{1}{2}} + 16830000i(-3iF_0)^{\frac{1}{2}}},
\]

(7.38)

\[
c_2 = \frac{1683F_0 + 1417iF_0}{20000(-3iF_0)^{\frac{1}{2}}},
\]

(7.39)

Component c \((F_{1c})\): 6th harmonic

Similarly, \( F_{1c} \) can be written as

\[
F_{1c} = D(\eta, \tau) \sin(6T) + E(\eta, \tau) \cos(6T).
\]

Defining \( J = D + iE \), the following equation and boundary conditions are obtained:

\[
F_0^3 J_{\eta \eta \eta \eta} + 6iJ = 0; 
\]

(7.40)

\[
J_{\eta}(0, \tau) = -7A^2 s \sin(7A) + i\left(\frac{A^2}{2}(\cos(7A))^2 + 7A^2 \cos(7A)\right)s, \quad J_{\eta \eta \eta \eta}(0, \tau) = 0. 
\]

(7.41)

Also, for matching, \( J \) must remain bounded as \( \eta \to \infty \). With \( J \) determined, \( F_{1c} \) is given by:

\[
F_{1c} = c_3 e^{-\frac{1}{F_0}(-6iF_0)^{\frac{1}{2}} x} + c_4 e^{-\frac{1}{F_0}(-6iF_0)^{\frac{1}{2}} x}, 
\]

(7.42)
where $c_3$ and $c_4$ are both constants. Their values are

$$
c_3 = \frac{631657F_0}{9920000(-6iF_0)^{3/4} - 12420000(-6iF_0)^{3/4},}
$$

$$
c_2 = \frac{496F_0 - 621iF_0}{20000(-6iF_0)^{3/4}},
$$

The analytical solution in the boundary layer is plotted and compared with the numerical solution in Figure 7-3 for $A = 0.1$ and $\omega = 10^4$.

### 7.2.4 Effective slope condition for outer solution

Recall that the evolution of the leading-order outer film height $H_0(\xi, \tau)$ satisfies

$$
H_0 + (H_0^3 H_{0\xi\xi\xi})_\xi = 0; \tag{7.45}
$$

$$
H_{0\xi\xi}(0) = 0, \quad H_{0\xi\xi}(1, \tau) = H_{0\xi}(1, \tau) = 0. \tag{7.46}
$$

To obtain the remaining boundary at the origin, Van Dyke's rule is applied, yielding:

$$
H_{0\xi}(0, \tau) = -s(1 - 7A^2 \cos(7A) + \frac{A^2(\cos(7A))^2}{2}). \tag{7.47}
$$

Using (7.45) - (7.47), the outer solution $H_0$ can be obtained numerically. This numerical solution together with the inner solution is compared to the full numerical solution in Figure 7-3.

### 7.3 Discussion

Figure 7-3 compares the theoretically and numerically obtained solutions for $H$ and $P$. Clearly, the theoretical outer solution overlaps with numerical solution very well except in a small region near the corner, which is the boundary layer and is governed by the inner solution. An advantage of simulating the outer equations that it requires much less computational time than does the full numerical solution. The reason is that the stretching term is absent from the outer equation. Thus, in this large-frequency stretching scenario,
Figure 7-3: High-frequency stretching: comparison of theoretical and numerical $h(x, t)$ (top) and $p(x, t)$ (bottom) profiles for $A = 0.1$, $\omega = 10^4$, $d = 0.01$ after 60 cycles.
the code used to compute the outer solution can be used in lieu of the original stretching code in order to reduce the computation time. From a physical viewpoint, the outer region is controlled by kinematic stretching and by the effective slope boundary condition provided by the inner solution.

According to the analysis, the width of boundary layer is $O(\omega^{-\frac{1}{2}})$. Figure 7-3 is obtained by setting $\omega = 10^4$, which implies a boundary layer width that is $O(0.1)$. This conclusion matches Figure 7-3 very well, for the inner solution almost overlaps with the numerical solutions for $x < 0.1$. Recall from Chapter 2 that a Gaussian curvature term is imposed near the corner in order to obtain a smooth pressure profile. As it decays exponentially it will only affect $H$ and $P$ within $x = O(d)$. Here, $d = 0.01$, and the inner solution differs with the numerical results when $x < 0.01$, in agreement with Figure 7-2.

The pressure profile obtained from the inner solution should be the same as that of numerical solution when $0.1 < x < 0.5$; this is why the right-hand-side of Figure 7-3 only shows the $x$ axis from 0.1 to 0.5. However, these two curves do not overlap with each other even though they have a similar shape. One explanation for this discrepancy is that there may be an $O(1)$ mean contribution to the pressure that arises from the $O(\omega^{-\frac{1}{2}})$ terms, neglected in the analysis. Thus, in order to improve the accuracy, the third term in the perturbation expansion should be computed.

Figure 7-4 shows the theoretical pressure profile near the corner. It correctly captures the large pressure fluctuations near the corner, which could be important for alveolar structural stability and capillary blood flow. Therefore, this high frequency scenario is potentially important to clinical research.
Figure 7-4: Theoretical pressure distribution near the corner for \( A = 0.1, \omega = 10^4 \) after 60 cycles. Compare with curves 1 and 5 in the lower plot of Figure 7-1.
CHAPTER 8

SMALL-AMPLITUDE STRETCHING AT $O(1)$ FREQUENCY

As there are no high resolution medical devices that can yet accurately image in vivo alveolar kinematics, it is sensible to investigate a broad parameter regime to investigate the range of possible physical phenomena. In this chapter, the redistribution of the liquid film caused by small-amplitude stretching at $O(1)$ frequency is studied.

8.1 Numerical Results

Figure 8-1 and Figure 8-2 show the film height and pressure profiles computed for $A = 0.1$ and $\omega = \frac{2\pi}{0.1}$ after 40 cycles in Lagrangian and Eulerian variables, respectively. Unlike Figure 7-1 and Figure 7-2, the pressure profiles here suggest that a wave-like disturbance is introduced near the corner and then propagates along the puddle to the contact point, where it is largely reflected. To capture this pressure feature, the following analysis focuses on the puddle region near the contact point. Beyond the contact point, the droplet again exhibits only kinematic (mass-conserving) changes.
Figure 8-1: Lagrangian film height (top) and pressure (bottom) distributions during 40th cycle. $A = 0.1, \omega = \frac{2\pi}{0.1}, (d = 0.05.)$
Figure 8-2: Eulerian film height (top) and pressure (bottom) distributions during 40th cycle.

\[ A = 0.1, \omega = \frac{2\pi}{0.1} \quad (d = 0.05) \]
8.2 Theoretical Analysis

Since $A$ is a small parameter, while $\omega$ is fixed and $O(1)$, the governing thin film equation is linearized about the quasi-static puddle solution. Again, it proves advantageous to carry out the analysis in Lagrangian variables. Substituting $H = H_0 + AH_1$ into the model thin film equation yields:

\[
(H_0 + AH_1)_{\tau} + [(H_0 + AH_1)^3(H_0 + AH_1)_{\xi\xi}]_{\xi} = 0,
\]

where, as introduced previously, $\tau$ is a new time variable that satisfies $\frac{dT}{dt} = \frac{1}{3\omega}$. Meanwhile, the inhomogeneous slope boundary condition becomes:

\[
H_\xi(0^+, t) = -s(1 + A\sin(\omega t))^2 = -s - 2sA\sin(\omega t) - sA^2(\sin(\omega t))^2. \tag{8.2}
\]

Substituting the relationship between $\tau$ and $t$:

\[
\tau = \int_0^t \frac{dt}{3(1 + A\sin(\omega t))^2} \sim \frac{1}{3} \int_0^t [1 - 7A\sin(\omega t) + O(A^2)]d\tilde{t} = \frac{1}{3} + \frac{7A}{3\omega} [\cos(\omega t) - 1] + O(A^2).
\]

Therefore,

\[
t \sim 3\tau - \frac{7A}{\omega} [\cos(3\omega \tau) - 1] + O(A^2). \tag{8.4}
\]

For small $A$, boundary condition (8.2) can be expressed as:

\[
H_\xi(0^+, \tau) \sim -s - 2sA\sin(3\omega \tau) + O(A^2). \tag{8.5}
\]

At $O(A^0)$,

\[
H_0\tau + [H_0^3H_{0\xi\xi}]_{\xi} = 0, \tag{8.6}
\]

subject to the following approximate boundary conditions on the puddle region:

\[
H_0(0^+, \tau) = -s, \quad H_0\xi(0^+, \tau) = 0, \quad H_0\xi(x_c, \tau) = H_0(x_c, \tau) = 0, \tag{8.7}
\]

where $x_c$ is the location of the contact point. In a quasi-steady state, the leading-order solution is parabolic:

\[
H_0 = \frac{s}{2x_c} \xi^2 - s\xi + \frac{s}{2} x_c. \tag{8.8}
\]
Introducing a new coordinate \( \eta = x_c - \xi \) whose origin is the contact point, \( H_0 \) can be recast as

\[
H_0 = \frac{s\eta^2}{2x_c}. \tag{8.9}
\]

At \( O(A) \),

\[
H_{1r} + [H_0^3 H_1 \xi \xi \xi] \xi = 0 \tag{8.10}
\]

subject to

\[
H_{1c}(0, \tau) = -2s \sin(3\omega \tau), \quad H_{1 \xi \xi \xi}(0^+, \tau) = 0, \quad H_1(x_c, \tau) = 0, \quad H_{1 \xi}(x_c, \tau) = 0. \tag{8.11}
\]

However, as the analysis that follows is applicable only near \( x_c \), the boundary conditions at \( \xi = 0 \) cannot be explicitly imposed. To solve the above linear but non-constant coefficient equation for \( H_1 \), set \( H_1 = \tilde{H}(\eta)e^{i\omega \tau} + c.c. \), where \( c.c. \) denotes complex conjugate, then:

\[
i\omega \tilde{H}_1 + [H_0^3 \tilde{H}_{1 \eta \eta \eta}] \eta = 0, \tag{8.12}
\]

or

\[
i\omega \tilde{H}_1 + H_0^3 \tilde{H}_{1 \eta \eta \eta} + 3H_0^2 \dot{H}_0 \tilde{H}_{1 \eta \eta} = 0. \tag{8.13}
\]

Restricting attention to a region localized near \( x_c, \eta \ll 1 \). Thus, it is convenient to rescale \( \eta \) by defining \( \eta = \epsilon \chi \) where \( \chi \) is an \( O(1) \) variable and \( \epsilon \) is a small (positive) parameter. Substituting into (8.13) yields

\[
\frac{i8\omega x_c^3}{s^3 \lambda^6} \tilde{H}_1 + \epsilon^2 \tilde{H}_{1 \chi \chi \chi} + \epsilon^2 \frac{6}{\chi} \tilde{H}_{1 \chi \chi} = 0. \tag{8.14}
\]

The WKB method can be used to solve this problem. For simplicity, define the constant

\[
a = \frac{is\omega(x_c)^3}{s^3}. \tag{8.15}
\]

Assuming \( \tilde{H}_1 \sim \epsilon^{\frac{1}{2}} \sum_{n=0}^{\infty} (\delta^n \eta_n(\chi)) \), then:

\[
\tilde{H}_{1 \chi \chi \chi} \sim \frac{3}{s^2} \left( \sum_{n=0}^{\infty} (\delta^n \eta'_n)) \right) \left( \sum_{n=0}^{\infty} (\delta^n \eta''_n) \right) + \frac{1}{s} \left( \sum_{n=0}^{\infty} (\delta^n \eta'''_n) \right) + \frac{1}{s^3} \left( \sum_{n=0}^{\infty} (\delta^n \eta'_n)^3 \right) + \frac{\epsilon^{\frac{1}{2}}}{\sum_{n=0}^{\infty} (\delta^n \eta_n(\chi))},
\]

where ' means the derivative of \( \chi \). Similarly,
To obtain the first two WKB terms $S_0, S_1$, it is only necessary to retain the $O(\frac{1}{\delta^4})$ and $O(\frac{1}{\delta^3})$ terms after substituting into (8.14):

\[
\frac{\varepsilon^2}{\delta^4} (S_0')^4 + \frac{6 \varepsilon^2}{\delta^3} (S_0')^2 S_0'' + \frac{4 \varepsilon^2}{\delta^3} S_0' (S_0')^3 + \frac{a}{\chi^3} + \frac{6 \varepsilon^2}{\delta^3} (S_0')^3 = 0. \tag{8.16}
\]

Recalling $\varepsilon$ and $\delta$ are both small parameters, the above equation indicates their relationship:

\[
\varepsilon^2 = \delta^4. \tag{8.17}
\]

Then the leading order equation is

\[
(S_0')^4 = -\frac{a}{\chi^3}, \tag{8.18}
\]

while at next order,

\[
3S_0'' + 2S_0'S_1' + \frac{3}{\chi} S_0' = 0. \tag{8.19}
\]

From (8.18), $S_0'$ clearly will have four roots. To ensure that $H_1$ will not be exponentially large as $\chi \to 0^+$, $S_0$ should have a negative real part. In other words, only two roots of $S_0'$ can be kept, as discussed later in this chapter.

Whatever roots are chosen, the solution of $S_0'$ can be written as $b \chi^{-\frac{3}{2}}$ where $b$ is a known constant. Then

\[
S_0 = -2b \chi^{-\frac{1}{2}} + C_1, \tag{8.20}
\]

where $C_1$ is an undetermined constant. Substituting (8.20) into (8.19) and integrating gives

\[
S_1 = \frac{3}{4} b \ln \chi + C_2, \tag{8.21}
\]

where $C_2$ is also an undetermined constant.

Recalling that $\varepsilon = \delta^2$ and $\eta = \varepsilon \chi$, the perturbation to the parabolic film height can be expressed as
\[
H_1 = A e^{-\frac{2b}{\sqrt{\eta}}} + \frac{C_1 + \frac{3}{4} \ln(\eta) - \frac{3}{4} \ln(\epsilon) + C_2 e^{i\omega \tau} + c.c.}{\epsilon}
\]

(8.22)

Since \( \epsilon, C_1 \) and \( C_2 \) are all constants, they can be incorporated into \( \tilde{A} \) (which should not be confused with the stretching amplitude \( A \) defined previously). Therefore,

\[
H_1 = a \eta^{\frac{3}{2}} e^{-\frac{2b}{\sqrt{\eta}}} e^{i\omega \tau} + c.c.,
\]

(8.23)

where \( a \) is the (complex) solution amplitude. To ensure this solution will not blow up as \( \eta \to 0^+ \), the roots represented by \( b \) should have positive real part, where

\[
b = (-i)^{\frac{1}{4}} \left( \frac{8 \omega x^3}{\xi} \right)^{\frac{1}{4}}.
\]

(8.24)

Of the four roots, only two have positive real part. These are retained in the \( H_1 \) solution, which then can be written as a superposition of two terms:

\[
H_1 = [A_1 e^{-\frac{2b}{\sqrt{\eta}}} + A_2 e^{-\frac{2b}{\sqrt{\eta}}}] \eta^{\frac{3}{4}} e^{i\omega \tau} + c.c.,
\]

(8.25)

where \( A_1 \) and \( A_2 \) are the complex amplitudes and \( r_1 = e^{i\frac{3\pi}{8}} \left( \frac{8 \omega x^3}{\xi} \right)^{\frac{1}{4}} \), \( r_2 = e^{-i\frac{3\pi}{8}} \left( \frac{8 \omega x^3}{\xi} \right)^{\frac{1}{4}} \).

### 8.3 Discussion

Figure 8-3 compares the numerical and WKB profiles of \( h(x,t) \) and \( p(x,t) \) after 40 cycles for \( A = 0.1 \), and \( \omega = \frac{2\pi}{60} \). Since the linear, homogeneous WKB analysis leaves \( A_1 \) and \( A_2 \) undetermined, these amplitudes are found by nonlinear least squares curve fitting with the numerical solution. The algorithm is as follows. First, the pressure distribution obtained from the numerical simulation is plotted. Then using Matlab's built-in function "lsqnonlin", a nonlinear least squares fitting is performed to obtain the values of \( A_1 \) and \( A_2 \) that enable the WKB pressure profile to most closely match its numerical counterpart over the region \( 0.3 < x < 0.5 \). In this way, \( A_1 \approx 2.9136 \) and \( A_2 \approx 872.4097 \). Finally, the WKB pressure profile is plotted using the known \( A_1, A_2 \) values and compared with the numerical pressure profile.
Figure 8-3: Comparison of numerically-computed and WKB profiles of $h(x,t)$ (top) and $p(x,t)$ (bottom) after 40 cycles. $A = 0.1$, $\omega = \frac{2\pi}{0.1}$. 

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The top plot in Figure 8-3 reveals a discrepancy between the numerical and WKB $h(x,t)$ profiles. This is because the analysis assumes the minimum liquid height at the contact point is zero; in the numerics, however, the minimum film height at the contact point has a finite value. Shifting the WKB curve to match the numerical solution at the contact point improves the agreement between these solutions.

Similarly, the WKB pressure profile does not agree quantitatively with the numerical solution. This discrepancy, too, may be caused by assuming minimum film height is zero. In addition, to carry out the nonlinear least squares fitting, equal weighting was given to the numerical solution values at all grid points from $0.3 < x < 0.5$, for fitting the WKB analytical solution. But considering this WKB solution captures the pressure profile better as long as the grid points are closer to the contact point, the numerical solution at grid points near the contact point should be given a much larger weight factor during nonlinear least squares fitting. Thereafter, the WKB pressure profile may be much closer to the numerical pressure profile. Nevertheless, the WKB and numerical pressure distributions have broadly similar features, suggesting that the linearized analysis captures the key physics in this stretching parameter regime: a pressure wave propagates from the corner along the puddle and is largely reflected at the contact point.
In order to explore the behavior of the thin liquid film that coats alveolar septa, a simplified mathematical model is investigated. The influences of corner geometrical features, periodic substrate stretching (to mimic respiration) and small liquid volumes (leading to an effective contact point along the substrate) are studied, extending earlier analyses of the alveolar liquid lining. The focus of this research is on understanding the competition between substrate stretching and capillary pressure variations in controlling the readjustment of the film. Lubrication theory is used to simplify the Navier-Stokes equation and to motivate the form of the model thin-film equation used in this investigation. Finite difference numerical simulations are used to explore the film dynamics captured by the highly nonlinear, fourth-order partial differential governing equation as the amplitude \((A)\) and frequency \((\omega)\) of stretching are varied. Asymptotic analysis is employed to gain insight into the dominant physical mechanisms in different regions of \(A-\omega\) parameter space.

According to the numerical results, the film distribution under periodic stretching depends on the initial liquid volume, the duration of stretching and the stretching amplitude and frequency. Two simple examples are studied first. The so-called Hammond problem that arises without stretching and the case of uni-directional extension are discussed and analyzed in detail to provide clues into the fluid distribution under periodic stretching. It is found that certain small scale regions, such as the Hammond Bretherton regions, arise. These regions play an important role in controlling fluid fluxes along the substrate.

After studying these two simple cases, periodic stretching scenarios with different stretching protocols are investigated. Aided by the numerical results, various asymptotic approxi-
mations are employed to derive new governing equations describing the dominant physical balances in different parts of the film.

Under low-frequency stretching, three interior regions (Bretherton, Wedge and Hammond) separate the corner puddle from the droplet. The Bretherton and wedge regions appear as a bifurcation from the no-stretching scenario as the stretching amplitude is increased for a given, small stretching frequency. These regions, which also appear in unidirectional extension, control the flux of fluid into and out of the corner. Interestingly, the analytical solution in the wedge region reveals a stretching wave. Also, the pressure profile observed in the Bretherton region is non-monotonic during contraction. The simulation of the extension and contraction process shows a net flux difference during one stretching cycle, which may account for the wedge width changing with time. Although the analysis suggests the wedge region is formed by net flux deposition at the end of the puddle region, the numerical results oppose this conclusion. Further research is required to understand the physics of film redistribution during one cycle in this parameter regime.

Under high-frequency, moderate-amplitude stretching, a boundary layer is found near the corner, which screens the film away from the corner from non-kinematic stretching effects. The boundary layer provides a fixed slope to the outer fluid distribution, which satisfies a quasi-steady problem without stretching in Lagrangian (substrate-fixed) variables. In addition, the magnitude of the pressure fluctuations near the corner reaches \( O(\omega^{\frac{1}{2}}) \), which may be important clinically since large pressure variations could influence alveolar structural stability and capillary blood flow.

When the substrate is stretched at small amplitude and \( O(1) \) frequency, the numerical results show that a capillary wave propagates along the puddle between the corner and contact point. This process is adequately captured by a WKB approximation. The analytical liquid film height and pressure solutions match the numerical solutions fairly well, considering the error incurred by assuming \( H_{\min} \) is zero at the contact point. Downstream of the contact point, the film is controlled by kinematic substrate stretching effects.

Figure 9-1 (compare with Figure 4-5) summarizes these conclusions and emphasizes
that, in different parameter regions, there will be different physical mechanisms governing the fluid re-distribution driven by the competition between capillary pressure variations and substrate stretching.

![Diagram](image)

Figure 9-1: Summary of dominant physical processes in different regions of $A-\omega$ parameter space investigated in this study.

In summary, this thesis presents an idealized model of the movement of the alveolar liquid lining. A mathematical model is developed to predict the fluid response to stretching. Various analytical methods, guided by the results of numerical simulations, are employed to discover the physical mechanisms that govern the fluid re-distribution under different stretching scenarios.

Future work includes properly treating larger interfacial curvatures in the corner, identifying the locations of bifurcations in $A-\omega$ parameter space, allowing for fully two-way coupling between the substrate motion and liquid film dynamics, and developing an advanced
model including Marangoni stresses associated with non-uniform surfactant distributions.
BIBLIOGRAPHY


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