INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6” x 9” black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.

UMI

A Bell & Howell Information Company
300 North Zeeb Road, Ann Arbor MI 48106-1346 USA
313/761-4700 800/521-0600
RICE UNIVERSITY

INSTABILITIES IN HEATED FALLING FILMS: A FULL-SCALE DIRECT NUMERICAL SIMULATION

by

Sivaramakrishnan Krishnamoorthy

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE

Doctor of Philosophy

APPROVED, THESIS COMMITTEE:

Bala Ramaswamy
Dr. Bala Ramaswamy, Chairman
Assistant Professor of Mechanical Engineering and Materials Science

Dr. Alan J. Chapman
Professor of Mechanical Engineering and Materials Science

Dr. John E. Akin
Professor of Mechanical Engineering and Materials Science

Dr. Dandy C. Sorensen
Professor of Computational and Applied Mathematics

Houston, Texas

May, 1996
INSTABILITIES IN HEATED FALLING FILMS: A FULL-SCALE DIRECT NUMERICAL SIMULATION

Sivaramakrishnan Krishnamoorthy

Abstract

A thin liquid layer draining on a heated inclined plane is susceptible to long surface waves, and can either form waves and stay continuous or go through a rupture process leading to the formation of rivulets. It is of great engineering significance to understand how various instability mechanisms decide the final state of the flow. In this regard, a numerical procedure has been developed to solve the governing equations for the conservation of mass, momentum, and energy. Temporal discretization is done using a Chorin-type projection scheme and the spatial discretization is done using the finite-element method in an Arbitrary Lagrangian Eulerian frame of reference.

The liquid layer is subjected to the thermocapillary instability when it is heated from below. When the layer is tilted, it drains downstream and can become unstable, even in the absence of heat transfer, due to surface-wave instability. When the layer is tilted and heated, both thermocapillary and the surface-wave instabilities coexist and dictate the dynamics of the flow in a competitive manner. The purpose of this study to gain further insight into the underlying instability mechanisms.

Through extensive numerical simulations, it is shown that in a horizontal layer, when the interfacial mode of thermocapillarity is dominant, the film always ruptures via fingering mechanism associated with the lubrication pressure. When the Pearson
mode of the thermocapillarity is dominant, the film stays continuous. In a vertical layer, the surface-wave instability is dominant and the film never ruptures and always stays continuous in the parametric range where long-wave theory is valid. For intermediate angles of inclination, rupture occurs for a disturbance with small enough wavenumber. A series of phase diagrams depicting the boundaries between wavy but continuous film and ruptured film are presented, and the interplay among instability mechanisms involved is examined. Lastly, formation of rivulets due to three-dimensional instabilities is studied in horizontal and vertical layers. A mechanism for rivulet formation, based on the instability phenomena, is discussed.
Acknowledgments

I sincerely thank my thesis advisor, Dr. Bala Ramaswamy, for his guidance, advice, and encouragement during this research. My special thanks to Dr. Sang Woo Joo, Wayne State University, Detroit, Michigan, for his guidance and advice. I would also like to thank Dr. John E. Akin, Dr. Alan Chapman and Dr. Danny Sorensen for serving on the dissertation committee.

The financial support by the Rice University and National Science Foundation is greatly appreciated. This research wouldn't have been possible without the excellent computational resources offered by the Department of Mechanical Engineering and Material Science at Rice University, NASA Lewis Research Center, Cleveland, Ohio, and Rice Advanced Visualization Laboratory, Rice University. I also sincerely thank my colleague Dr. Srinivas Chippada from whom I learned many aspects of research. My special thanks to my colleagues V. Ravi Rao and R. Moreno, with whom I had many fruitful discussions on the subject of this research.

Finally, I would especially thank my parents for their support, patience, and encouragement during these years while being far away from the home.
To my parents
# Nomenclature

<table>
<thead>
<tr>
<th>Symbols</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_n$</td>
<td>Fourier modes of surface wave</td>
</tr>
</tbody>
</table>
| $C$     | convection matrix  
  | also Courant number |
| $c$     | wave speed |
| $D$     | height of the cavity |
| $d$     | initial mean thickness of the film |
| $F, f$  | load vectors |
| $g$     | gravitational acceleration  
  | also grid-point velocity |
| $H$     | mean curvature of the interface |
| $h$     | height of the free surface  
  | also heat-transfer coefficient at the free surface |
| $k$     | wavenumber of the disturbance  
  | also thermal conductivity of the liquid |
| $L$     | length of two-dimensional computational domain  
  | also Laplacian or diffusion matrix |
| $M$     | mass matrix |
| $n$     | unit normal to the free surface |
| $N$     | shape function |
\( P \)  \quad \text{pressure matrix} \\
\( p \)  \quad \text{pressure} \\
\( Q \)  \quad \text{volumetric flow rate} \\
\( T \)  \quad \text{dimensional temperature} \\
\( t \)  \quad \text{time} \\
also \text{orthonormal tangential vector to the free surface} \\
\( U \)  \quad \text{velocity vector} \\
\( u \)  \quad \text{velocity component in the } x \text{-direction} \\
\( v \)  \quad \text{velocity component in the } y \text{-direction} \\
\( w \)  \quad \text{velocity component in the } z \text{-direction} \\
\( (x,y,z) \) \quad \text{Cartesian coordinates} \\
\( X \)  \quad \text{material coordinates} \\
\( x \)  \quad \text{spatial coordinates} \\
\( \dot{x} \)  \quad \text{referential coordinates} \\

**Greek Letters** \\
\( \alpha \)  \quad \text{thermal diffusivity} \\
\( \alpha, \beta, \gamma \) \quad \text{nodal number} \\
\( \beta \)  \quad \text{angle of inclination of the plate} \\
\( \text{coefficient of volumetric expansion} \) \\
\( \Gamma \)  \quad \text{linear growth rate} \\
\( \gamma \)  \quad d\sigma/dT \\
\( \Delta x, \Delta y, \Delta z \) \quad \text{spatial increment in } x, y, \text{ and } z \text{-directions} \\
\( \Delta T \)  \quad \text{temperature difference} \\
\( \Delta t \)  \quad \text{time increment} \\
\( \delta_{ij} \) \quad \text{Kronecker delta}
\( \epsilon \)  
small parameter in long-wave expansion

\( \mu \)  
dynamic viscosity

\( \nabla \)  
\((\partial/\partial x, \partial/\partial y)\), gradient operator

\( \nu \)  
kinematic viscosity

\( \rho \)  
fluid density

\( \sigma \)  
surface tension

\( \sigma_0 \)  
surface tension at reference temperature \( T_s \)

\( \sigma_{ij} \)  
stress tensor

\( \theta \)  
nondimensional temperature

\( \omega \)  
growth rate

**Subscripts**

\( c \)  
cut-off value

\( i, j, k \)  
directions of Cartesian coordinate

\( M \)  
for maximum linear growth

\( S \)  
ambient

\( t \)  
derivative with time

\( W \)  
wall quantity

\( (x, y, z) \)  
component of the referred quantity in \( x, y, \) and \( z \)-directions respectively

\( , i \)  
partial derivative w. r. t. \( x_i \)

**Superscripts**

\( L \)  
lumped quantity

\( n \)  
\( n \)-th time step

\( (x, y) \)  
component of the referred quantity in \( x, \) and \( y \)-directions respectively

\( * \)  
nondimensional quantity
fluctuating quantity

intermediate value

mean quantity

Nondimensional Numbers

$Bi$ Biot number $(hd/k)$

$G$ Galileo number or thickness parameter $(gd^3/\nu^2)$

$M$ Marangoni number $(\gamma \Delta T d/[2\mu \kappa])$

$P$ Prandtl number $(\nu/\alpha)$

$Ra$ Rayleigh number $(\beta g \Delta T D^3/[\nu \alpha])$

$Re$ Reynolds number $(Ud/\nu)$

$S$ Surface tension parameter $(\sigma_0 d/[3\rho \nu^2])$

$\Gamma$ Kapitza number $(\sigma/[3\rho(\nu^2 g)^{1/3}])$

Note: Only the most important symbols are listed above. The symbols are defined wherever possible in the text. Symbols are also subject to alteration on occasion.
# Table of Contents

Abstract ................................................................. ii
Acknowledgments ......................................................... iv
Nomenclature ............................................................. vi
List of Figures ............................................................. xiii
List of Tables ............................................................. xvi

1 Introduction .............................................................. 1
   1.1 Motivation ........................................................... 1
   1.2 Course of Study ..................................................... 2

2 Heated Falling Films .................................................. 5
   2.1 Introduction ........................................................... 5
   2.2 Thin-Film Dynamics .................................................. 6
   2.3 Governing Equations ............................................... 9
   2.4 Boundary Conditions ............................................... 14
   2.5 Linear Stability Analysis ......................................... 16
   2.6 Nonlinear Analysis ................................................. 23
      2.6.1 Long-Wave Evolution Equation ............................. 23
      2.6.2 Boundary-Layer Approximation ............................. 27
   2.7 Numerical Studies .................................................. 28

3 Numerical Scheme ..................................................... 30
   3.1 Introduction ........................................................... 30
   3.2 ALE Formulation ..................................................... 32
3.3 Fractional Step Method ............................................. 37
3.4 Spatial Discretization ................................................. 39
3.5 Free-surface Calculation ............................................ 41
3.6 Code Validation .................................................... 43

4 Rupture in Horizontal Layers ........................................ 49
  4.1 Introduction ....................................................... 49
  4.2 Governing Equations ............................................. 50
  4.3 Method of Analysis .............................................. 53
  4.4 Fingering Process via Long-Wave Evolution Equation .......... 57
  4.5 Fingering Process via Full-Scale Computation .................. 60
  4.6 Influence of Biot Number and M/P ............................... 65
  4.7 Thick Horizontal Layers: Pearson Mode Instability ............ 71
  4.8 Conclusion ...................................................... 74

5 Thermocapillary and Surface-wave Instability in Inclined Layers 75
  5.1 Introduction ....................................................... 75
  5.2 Method of Analysis .............................................. 77
  5.3 Combined Thermocapillary and Surface-Wave Instabilities .... 78
  5.4 Merging and Splitting Process ................................... 88
  5.5 Pearson Mode Instability ...................................... 96
  5.6 Concluding Remarks ........................................... 103

6 Rivulet Formation in Three-Dimensional Flows ....................... 105
  6.1 Introduction ..................................................... 105
  6.2 Method of Analysis ............................................. 107
  6.3 Horizontal Film ................................................. 109
  6.4 Vertical Film ................................................... 118
  6.5 Concluding Remarks ........................................... 129
7 General Conclusions

7.1 Conclusion .................................................. 130

7.2 Future Work .................................................. 132

Bibliography ...................................................... 134
List of Figures

2.1 Film Flow over a Long Inclined Plate ............................ 7
2.2 Physical Configuration of a Thin Film Flowing Down a Heated
Inclined Plate ......................................................... 10

3.1 Arbitrary Lagrangian Eulerian Description of the Flow ........ 34
3.2 Physical Configuration of the Benchmark Problem Suggested by De
Vahl Davis & Jones .................................................. 44
3.3 Validation of Free-Surface Calculation ................................ 48

4.1 Typical Finite-Element Mesh at the Time of Rupture in a
Horizontal Layer .................................................... 55
4.2 Grid-Independence Study for Full-Scale Computation ............ 56
4.3 Simulation of Rupture in a Horizontal Layer Through Spectral
Computation of Long-Wave Evolution Equation ..................... 59
4.4 Simulation of Rupture in a Horizontal Layer Through Full-Scale
Computation .......................................................... 62
4.5 Comparison of Fourier Modes Between Full-Scale Computation and
Spectral Computation of Long-Wave Evolution Equation During
Rupture ................................................................. 64
4.6 Influence of Biot Number on Rupture in Horizontal Layers ....... 68
4.7 Influence of $\frac{M}{f}$ on Rupture in Horizontal Layers. .......................... 70
4.8 Pearson-Mode Instability in a Thick Horizontal Layer. ......................... 72
4.9 Pearson-Mode Instability at Very High Intensity of Heating in a Horizontal Layer. .......................................................... 73

5.1 Influence of Angle of Inclination on Rupture. .................................... 81
5.2 Nonlinear Phase Diagram Obtained Using Full-Scale Computation That Shows the Influence of Angle of Inclination and Wavenumber on Rupture. .......................................................... 84
5.3 Evolution of a Horizontal Layer at Various Wavenumbers. .................... 86
5.4 Evolution of a Vertical Layer at Various Wavenumbers. ....................... 88
5.5 Linear Stability Diagram: Influence of Wavenumber in an Isothermal Flow. .............................................................................. 89
5.6 Evolution of an Inclined Layer at Various Wavenumbers. .................... 93
5.7 Splitting and Merging Process in Nonisothermal Flows. ....................... 95
5.8 Linear Stability Diagram: Influence of Film Thickness and Heating. .... 96
5.9 Nonlinear Phase Diagram Obtained Using Full-Scale Computation That Shows the Influence of Film Thickness and Intensity of Heating on Rupture. .......................................................... 98
5.10 Evolution of an Inclined Layer at Various Intensity of Heating. .......... 100
5.11 Evolution of an Inclined Layer at Various Film Thickness. ............... 102

6.1 Simulation of Rivulet Formation in a Horizontal Layer Through Full-Scale Computation and Spectral Computation of Long-Wave Evolution Equation. .......................................................... 115
6.2 Comparison of Energy Norms Between Full-Scale Computation and Spectral Computation of Long-Wave Evolution Equation During Rivulet Formation in a Horizontal Layer. .......................... 117

6.3 Simulation of Rivulet Formation in a Vertical Layer Through Full-Scale Computation and Spectral Computation of Long-Wave Evolution Equation for $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_z=0.5$, and $k_y=0.05$. ................................. 125

6.4 Comparison of Energy Norms Between Full-Scale Computation and Spectral Computation of Long-Wave Evolution Equation During Rivulet Formation in a Vertical Layer for $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_z=0.05$, and $k_y=0.05$. ................................. 126

6.5 Simulation of Rivulet Formation in a Vertical Layer Through Full-Scale Computation for $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_z=0.05$, and $k_y=0.025$. ................................. 128
List Of Tables

3.1 Comparison of Thermal and Flow Quantities with Benchmark
Solutions of De Vahl Davis for \( Ra=10^3 \) ................................. 45

3.2 Comparison of Thermal and Flow Quantities with Benchmark
Solutions of De Vahl Davis for \( Ra=10^4 \) ................................. 46

3.3 Comparison of Thermal and Flow Quantities with Benchmark
Solutions of De Vahl Davis for \( Ra=10^5 \) ................................. 46

3.4 Comparison of Thermal and Flow Quantities with Benchmark
Solutions of De Vahl Davis for \( Ra=10^6 \) ................................. 47

4.1 Rupture Time in a Horizontal Layer Computed Using Full-Scale
Computation. ................................................................. 70
Chapter 1

Introduction

1.1 Motivation

The flow of a liquid layer on a solid substrate has many significant engineering applications in material processing, biomedical engineering, nuclear, aerospace and chemical industries. Some of the applications of technological importance are tertiary oil recovery; processes associated with multi-phase flow through porous media; spreading of liquid as in coating process; coalescence of drops and bubbles in foams and emulsion; fabrication of chips in micro electronics; study of cancer cells; development of anti-icing system for aircraft wings. The study of the thin-film stability is critical to the understanding of the physics of the problem that is common to all these areas.

The most widely observed phenomena in thin-film flows such as formation of transverse roll waves on the surface of the liquid, longitudinal roll patterns, wave breaking, rupture, breaking of a stream of liquid into independent rivulets, evaporation and termination of liquid layer at a contact line and the formation of dry spots, are caused by the interfacial-instability mechanism. Various hydrodynamic forces such as hydrostatic pressure, surface tension, thermocapillarity, and inertia of the mean flow interact with each other nonlinearly and play a decisive role in determining the final state of the system.

A heated falling film becomes unstable in the presence of long surface disturbances. The disturbances are regular and bounded. However, there may be certain
conditions under which they grow to a saturated state where the film stays continuous or to a catastrophic state where the film ruptures and forms rivulets. From a mathematical perspective, the catastrophic behavior may be considered as a breakdown of the model describing the system. The motivation for studying this problem is to gain an understanding of the instability mechanism and to study the subsequent flow development. An analysis of this nature is of help in controlling unstable flows. However, there are some applications where unstable flows are preferred over stable flows. For example, experimental observations have shown that in almost all cases of practical interest, the draining liquid layer displays random waves at the interface that enhance heat- and mass-transfer rates (Chu & Dukler, 1974). Hence in film-cooling operation, the waviness of the surface may be desirable for heat-transfer enhancement, but rupture can be disastrous.

In recent years, due to the tremendous progress achieved in computer architecture and computational algorithms, Computational Fluid Dynamics (CFD) has become a powerful tool to analyze various flow problems. It can be used not only to simulate problems of practical interest but also in understanding the flow phenomena of a theoretical nature. In this dissertation, a numerical model that uses finite-element method (FEM) is developed to study thin-film flow phenomena.

1.2 Course of Study

In this dissertation, a thin liquid layer draining on a heated inclined plane is considered. It is subjected to both surface-wave and thermocapillary instabilities. The nonlinear interaction between these two instability mechanisms may result in a continuous, but wavy film or a ruptured film. Rupture occurs in two stages: a thinning process followed by a spontaneous rupture. The dynamics of the wave formation and the thinning process are analyzed by solving the hydrodynamic equations for
mass, momentum, and energy conservation. Actual breaking occurs only when the thickness of the layer becomes less than 1000 Å. Beyond this point, molecular forces become significant and the governing equations become inadequate in describing the physics of the ensuing flow. Hence, in the present study, rupture is assumed when thickness becomes less than 1000 Å at which moment the computation will be stopped.

Chapter 2 discusses the dynamics of a liquid layer draining on a heated inclined plane. The governing equations and the boundary conditions are explained in detail. The important nondimensional parameters arising in these flows are outlined along with their significance.

A variety of nonlinear dynamics of these flows has been studied using either hydrodynamic stability analysis or a weakly-nonlinear analysis. However, toward incipient rupture the flow becomes highly nonlinear and neither of these methods of analysis are appropriate in modeling the system. Therefore, direct numerical simulation is used in the present study. The biggest challenge in the numerical simulation of moving-boundary problem is locating the free boundary. It is usually unknown and has to be calculated as part of the solution procedure. In this aspect, we use an Arbitrary Eulerian Lagrangian (ALE) frame of reference and integrate the governing equations using a finite-element method based on Chorin-type splitting algorithm. The details of the numerical scheme are explained in Chapter 3.

In a horizontal layer, thermocapillarity is the primary instability mechanism. There are two modes of thermocapillarity: the interface mode and the Pearson mode. The dynamics of these modes are discussed in Chapter 4. Here, we show that the film always ruptures when the interfacial mode is dominant and stays continuous when the Pearson mode is dominant.
When the layer is tilted, it drains downstream and can become unstable even in the absence of heat-transfer. This isothermal mode of instability is called surface-wave instability. When the layer is tilted and heated, both surface-wave and thermocapillary instabilities coexist and dictate the dynamics of the flow in a competitive manner. When the thermocapillary instability is dominant the film always ruptures while the surface-wave instability is dominant, the film always stays continuous. In Chapter 5, the influence of various control parameters, such as the film thickness, spatial dimension of the disturbance, intensity of heating and the heat loss at the interface, on the combined instability mechanism is systematically studied. A series of nonlinear phase diagrams that depict the boundaries between the final states, a continuous film or a ruptured film, is also presented.

The final task is to understand the effect of thermocapillary and surface-wave instabilities in a three-dimensional system. In this regard governing equations along with nonlinear free-surface conditions are solved in three-dimensions in Chapter 6. Formation of rivulets in both horizontal and vertical layers is examined. Finally, some general conclusions and future research directions are discussed in Chapter 7.
Chapter 2

Heated Falling Films

2.1 Introduction

A wave is a disturbance that propagates from one place to another. In the simplest form, it is linear, nondissipative, and nondispersive. It is characterized by a wavelength that describes the spatial dimension and a frequency that describes the temporal dimension. In a heated falling film, waves are generated at the interface due to the presence of mean flow, and are enhanced by thermocapillarity. The final state of the flow is solely determined by the outcome of the nonlinear interplay between the destabilizing forces such as inertia and thermocapillarity and the stabilizing forces such as hydrostatic pressure and surface tension.

In thin-liquid layers, surface tension suppresses the disturbances of short wavelength and hence, the instability occurs in the form of long surface waves. The unstable layer exhibits corrugations at the interface and shows various wave motions. These waves are purely two-dimensional near inception and develop into a nonlinear saturated state as they drain downstream. They continue to grow and finally become chaotic and three-dimensional (Chang, 1994). However, in a heated layer, the dynamics are much more intriguing due to the presence of thermocapillarity. In this case, the layer either form waves and stay continuous or break and form rivulets. In this chapter, the thin-film flow phenomena, the equations that govern these flows, and the boundary conditions are discussed. A brief review on
linear and weakly nonlinear theories is presented. Finally, recent efforts in full-scale computation are discussed.

2.2 Thin-Film Dynamics

Consider a thin layer of liquid draining down a plane inclined at an angle $\beta$ to the horizontal. Define a Reynolds number ($Re$) based on the average velocity, average film thickness and the kinematic viscosity of the fluid. When $Re$ is low, $Re<3\csc\beta$ (Yih, 1963), the flow is smooth and parallel, and has a parabolic velocity profile, called Nusselt film flow. As the Reynolds number increases, the flow becomes unstable and ripples appear at the interface. Further increase in $Re$ leads to the formation of roll waves whose amplitude may be as large as the thickness of the film. These waves can be either laminar or turbulent depending on the value of $Re$. For $Re$ above 1500, the flow becomes stochastic and turbulent (Lin & Wang, 1985).

In a thin layer draining down a long inclined plane, various zones can be identified as shown in Fig. 2.1. Starting with the entrance region (zone 1) from reservoir downstream, in zone 2, the flow is smooth and parallel where the Nusselt thin-film flow solution is valid. Further downstream, in zone 3, smooth sinusoidal waves appear at the interface and in zone 4, they undergo a splitting and merging process. After the process of reorganization and coalescence, the roll waves, separated by a laminar film, appear in zone 5. Further downstream, in zone 6, the turbulent bursts are initiated and the transition process starts. The flow becomes fully turbulent with the emergence of turbulent roll waves in zone 7.

In a recent review, Chang (1994) identifies four distinct regions based on the nonlinear mechanism in the evolution process. In region I, that comprises of zones 1 to 3, the infinitesimal disturbances are amplified, grow exponentially and emerge as
monochromatic waves at the exit. If the inlet flow from the reservoir is artificially excited, for example pulsating the flow with a wire or a ribbon, the monochromatic waves inherit the forcing frequency. If the disturbances are broad-banded, a selective filtering process occurs in this region and still, monochromatic waves emerge at the exit. The stability of the flow in this region can be analyzed using a linear theory.

The region II overlaps zones 3 and 4. Here the exponential growth of the waves is arrested and the nonlinear mechanism becomes evident. The waves no longer maintain the sinusoidal profile, as the energy from the fundamental mode is transferred to its first harmonic. In a periodically forced experiment with large
amplitude waves, regions I and II may be bypassed and the wave field emerges with a large amplitude.

The region III comprises of zone 5. Here, the finite amplitude waves exiting region II are subjected to various types of instabilities such as subharmonic and sideband types. The waves split and merge consistently, their amplitudes grow and finally saturate to teardrop humps. These are also called solitary waves and have a sharp front end and a gently sloping tail. Small capillary ripples, called bow waves, travel ahead of these humps. Because of the shape, the waves are broad banded with superharmonics containing significant amount of energy.

The region IV comprises zones 6 and 7 where the turbulent bursts initiate and the flow undergoes a transition process. Transverse instabilities become dominant and the flow is no longer two-dimensional. It becomes chaotic and three-dimensional. The turbulent roll waves emerge from this region.

The above discussions are based on experimental observations in an isothermal flow where only the surface-wave instability is present. However, when the plate is heated, an additional mode of instability arises due to the thermocapillarity. The competition between these two instability mechanisms will decide the final state of the system. To study the dynamics, one can apply the linear theory in the region I only. Beyond this region, the nonlinearity becomes significant and the complete system of governing equations needs to be solved. Hence, in the present study, the conservation laws for mass, momentum and energy are solved in a fully coupled manner using a finite-element method. The governing equations are solved in both two and three-dimensions to study the rupture dynamics and rivulet formation.
2.3 Governing Equations

We consider a thin layer of constant density $\rho$, dynamic viscosity $\mu$, thermal conductivity $k$, thermal diffusivity $\alpha$, draining down a plate maintained at a constant temperature $T_w$ and inclined at an angle $\beta$ to the horizontal as shown in Fig. 2.2. It is unbounded in the streamwise and spanwise directions, but bounded above by the air with a far-field temperature $T_s(<T_w)$ and at zero pressure. The density and viscosity of the air are much smaller than those of the liquid, so that the dynamics of the air are decoupled from that of the liquid. With the flow downstream and the heat transfer, the liquid-air interface is free to deform. The heat transfer across the liquid layer is lost through the interface and determines the interfacial temperature $T_i$. We assume that the surface tension decreases linearly with temperature:

$$\sigma(T) = \sigma_0 - \gamma(T - T_s),$$  \hspace{1cm} (2.1)

where $\sigma_0$ is the surface tension coefficient at the reference temperature $T_s$ and $
\gamma(=-d\sigma/dT)$ is positive for most common liquids.

The flow is described by the time-dependent and three-dimensional conservation laws for mass, momentum and energy. Using the mean film thickness $d$, viscous time $d^2/\nu$, and temperature difference $(T_w - T_s)$, we write the following nondimensional quantities:

$$\begin{align*}
    & x^* = \frac{x}{d}; \quad y^* = \frac{y}{d}; \quad z^* = \frac{z}{d}; \quad t^* = \frac{t\nu}{d^2}; \\
    & u^* = \frac{ud}{\nu}; \quad v^* = \frac{vd}{\nu}; \quad w^* = \frac{wd}{\nu}; \quad \theta = \frac{T - T_s}{T_w - T_s};
\end{align*}$$  \hspace{1cm} (2.2)

where, $(u,v,w)$ are the components of the velocity vector in the streamwise $(x)$, spanwise $(y)$ and the vertical $(z)$ directions, respectively, and $\theta$ is the nondimensional temperature. The superscript "*" denotes their respective nondimensional quantities. Dropping "*" for convenience, we can write the governing equations as:
Figure 2.2: Physical configuration of a thin film flowing down a heated inclined plate.

Conservation of mass:
\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0,
\] (2.3)

Conservation of momentum:
\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + C \sin \beta + \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right),
\] (2.4)

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right),
\] (2.5)

\[
\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} - C \cos \beta + \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right),
\] (2.6)

Conservation of energy:
\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + w \frac{\partial \theta}{\partial z} = \frac{1}{P} \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2} \right),
\] (2.7)

where, \( p \) is the pressure, and
\[ G = \frac{d^2 g}{\nu^2}, \quad (2.8) \]

\( g \) is the gravitational acceleration, and \( gd^2 \sin \beta / \nu \) is the velocity at the interface in a uniform layer (see Eq. 2.38). \( G \sin \beta \) is analogous to the Reynolds number and it is also called as Galileo number in some literature. This parameter is a measure of film thickness. The Prandtl number

\[ P = \frac{\nu}{\alpha}, \quad (2.9) \]

is the ratio between the momentum diffusion to the thermal diffusion. We use a Cartesian coordinate system \( (x,y,z) \), with \( x \)-axis directed downstream, \( y \)-axis runs in the spanwise direction and the \( z \)-axis into the liquid from the bottom plate. The origin of the system is assumed located at the corner of the plate.

The liquid-air interface, \( z = h(x,y,t) \), changes in both streamwise and spanwise locations and with time. Here, we need to satisfy the kinematic, tangential- and normal-stress conditions, as well as the energy balance. The kinematic equation is defined as:

\[ \frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = w, \quad (2.10) \]

which states that the liquid particles at the interface move with the interface. The normal component of the surface traction is balanced by the capillary force

\[ \sigma_{ij} n_j n_i = 6HS, \quad (2.11) \]

which is surface tension times twice the mean curvature of the interface \( (H) \) where we have used the tensor notation to represent stress tensor \( \sigma_{ij} \) for clarity:

\[ \sigma_{ij} = -p \delta_{ij} + \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (2.12) \]
Here, \( u_i = (u, v, w) \) is the velocity vector, \( x_i = (x, y, z) \) is the Cartesian coordinates system, and \( \delta_{ij} \) is the Kronecker delta. The unit normal vector \( n_i \) is expressed as:

\[
(n_1, n_2, n_3) = \left( \frac{-\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, 1}{\sqrt{1 + \left( \frac{\partial h^2}{\partial x} + \frac{\partial h^2}{\partial y} \right)^{\frac{3}{2}}}} \right).
\]

Using the explicit expression for the curvature of the interface,

\[
H = \frac{1}{2} \frac{\partial^2 h}{\partial x^2} \left( 1 + \frac{\partial h^2}{\partial y} \right) - 2 \frac{\partial h}{\partial x} \frac{\partial h}{\partial y} \frac{\partial^2 h}{\partial x \partial y} + \frac{\partial^2 h}{\partial y^2} \left( 1 + \frac{\partial h^2}{\partial x} \right)
\left( 1 + \frac{\partial h^2}{\partial x} + \frac{\partial h^2}{\partial y} \right)^{\frac{3}{2}},
\]

the normal stress condition can be expressed as:

\[
-\rho + \frac{2}{N^2} \left[ \left( \frac{\partial^2 h}{\partial x^2} - 1 \right) \frac{\partial u}{\partial x} + \left( \frac{\partial h^2}{\partial y} - 1 \right) \frac{\partial v}{\partial y} \right]
- \frac{2}{N^2} \left[ \frac{\partial h}{\partial x} \left( \frac{\partial u}{\partial z} + \frac{\partial v}{\partial x} \right) + \frac{\partial h}{\partial y} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) - \frac{\partial h}{\partial x} \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \frac{\partial v}{\partial x} \right] = 6HS,
\]

where,

\[
N = \left( 1 + \frac{\partial h^2}{\partial x} + \frac{\partial h^2}{\partial y} \right)^{\frac{3}{2}}.
\]

The parameter

\[
S = \frac{\sigma_0 d}{3 \rho \nu^2},
\]

is the measure of surface tension. In the absence of viscosity, Eq. 2.11 is called the Laplace condition which states that the pressure is larger on the concave side of the interface by an amount \( 6HS \). Both \( G \) and \( S \) depend on the film thickness and can be related by a parameter

\[
\Gamma = \frac{\sigma}{3 \rho \nu^{4/3} g^{1/3}},
\]
so that \( S = \Gamma G^{1/3} \). This parameter, referred as Kapitza number in some literature, is a function of fluid properties alone. For a fixed \( \Gamma \), we can control the film thickness by varying \( G \). The shear stress at the interface is affected by the thermocapillarity, and is expressed as:

\[
\sigma_{ij} n_j t_i^x = -\frac{2M}{P} \frac{\partial \theta}{\partial x_i} t_i^x,
\]

(2.19)

\[
\sigma_{ij} n_j t_i^y = -\frac{2M}{P} \frac{\partial \theta}{\partial x_i} t_i^y,
\]

(2.20)

where, \( t_i^x \) and \( t_i^y \) are the orthonormal tangential vector to the free surface; \( t_i^x \) is parallel to the \( x \)-axis and \( t_i^y \) is parallel to the \( y \)-axis. Using the explicit expression for these vectors

\[
(t_1^x, t_2^x, t_3^x) = \frac{\left(1, 0, \frac{\partial h}{\partial x}\right)}{\left(1 + \frac{\partial h^2}{\partial x}\right)^{\frac{1}{2}}},
\]

(2.21)

\[
(t_1^y, t_2^y, t_3^y) = \frac{\left(0, 1, \frac{\partial h}{\partial y}\right)}{\left(1 + \frac{\partial h^2}{\partial y}\right)^{\frac{1}{2}}},
\]

(2.22)

the Eqs. 2.19 and 2.20 can be written as:

\[
\begin{align*}
\left(1 - \frac{\partial h^2}{\partial x}\right) \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) - 2\frac{\partial h}{\partial x} \left(2\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) - \frac{\partial h}{\partial y} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) - \\
\frac{\partial h}{\partial x} \frac{\partial h}{\partial y} \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right) = -\frac{2MN}{P} \left(\frac{\partial \theta}{\partial x} + \frac{\partial h}{\partial x} \frac{\partial \theta}{\partial y}\right),
\end{align*}
\]

(2.23)

\[
\begin{align*}
\left(1 - \frac{\partial h^2}{\partial y}\right) \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) - 2\frac{\partial h}{\partial y} \left(2\frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}\right) - \frac{\partial h}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) - \\
\frac{\partial h}{\partial x} \frac{\partial h}{\partial y} \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right) = -\frac{2MN}{P} \left(\frac{\partial \theta}{\partial y} + \frac{\partial h}{\partial y} \frac{\partial \theta}{\partial z}\right),
\end{align*}
\]

(2.24)
where Marangoni number
\[ M = \frac{\gamma \Delta T d}{2 \mu \alpha}. \quad (2.25) \]

The thermocapillary forces, introduced into the problem through the tangential stress balance, can alter the capillary pressure jump at a particular location and induce a surface flow from the hotter side of the interface to the colder end (for \( \gamma > 0 \)). The energy balance on the interface gives
\[ \frac{\partial \theta}{\partial x} n_i + Bi \theta = 0, \quad (2.26) \]
or more explicitly
\[ \frac{\partial h}{\partial x} \frac{\partial \theta}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial \theta}{\partial y} - \frac{\partial \theta}{\partial z} + Bi N \theta = 0, \quad (2.27) \]
where,
\[ Bi = \frac{hd}{k}, \quad (2.28) \]
is the Biot number and \( h \) is the heat-transfer coefficient at the interface. The Biot number determines the amount of heat loss at the free surface. The thermocapillarity does not occur if \( Bi=0 \) or \( \infty \). \( Bi=0 \) corresponds to an insulated free-surface and the interface obtains the plate temperature \( (T_w) \). On the other hand, \( Bi=\infty \) corresponds to a highly conductive fluid and the interface obtains the temperature of the ambient gas \( (T_s) \).

### 2.4 Boundary Conditions

The governing equations, Eqs. 2.3 to 2.7, are solved in a three-dimensional domain of size \( L_x, L_y, \) and \( h(x,y,t) \) where
\[ L_x = \frac{2\pi}{k_x}, \quad (2.29) \]
and
\[ L_y = \frac{2\pi}{k_y}. \quad (2.30) \]

Here \( k_x \) and \( k_y \) are the disturbance wavenumber in the streamwise and spanwise directions. A spatial periodic boundary condition is applied for the variables \( u, v, w, p, \) and \( \theta \).

\[
\begin{align*}
  u(0, y, z, t) &= u(L_x, y, z, t); & u(x, 0, z, t) &= u(x, L_y, z, t); \\
  v(0, y, z, t) &= v(L_x, y, z, t); & v(x, 0, z, t) &= v(x, L_y, z, t); \\
  w(0, y, z, t) &= w(L_x, y, z, t); & w(x, 0, z, t) &= w(x, L_y, z, t); \\
\end{align*}
\]  
\quad (2.31)

\[
\begin{align*}
  p(0, y, z) &= p(L_x, y, z); & p(x, 0, z) &= p(x, L_y, z); \\
  \theta(0, y, z) &= \theta(L_x, y, z); & \theta(x, 0, z) &= \theta(x, L_y, z); \\
\end{align*}
\]  
\quad (2.32)

On the plate no-slip
\[
\begin{align*}
  u(x, y, 0, t) &= 0; \\
  v(x, y, 0, t) &= 0; \\
  w(x, y, 0, t) &= 0; \\
\end{align*}
\]  
\quad (2.33)

and constant temperature
\[ \theta(x, y, 0, t) = 1, \quad (2.34) \]

boundary conditions are applied. At the liquid-air interface, the normal-stress (Eq. 2.15), tangential-stress (Eqs. 2.23 and 2.24) conditions and the energy balance (Eq. 2.27) are applied. In the numerical procedure, the normal stress condition is directly incorporated into the momentum equations, while the tangential stress balance is applied as a natural boundary condition. In this problem, we have six unknown variables, \( u, v, w, p, \theta, \) and \( h \), to solve with the help of six equations, \( x, y, \) and \( z \)-momentum equations, continuity equation, energy equation, and the kinematic condition.
2.5 Linear Stability Analysis

This methodology requires a base-flow solution on which the stability analysis is performed. In thin-film flows, the Nusselt-flow solution is usually considered as a base flow. This is arrived at as follows: Consider a layer draining on a plate inclined at an angle $\beta$ in the streamwise direction. The flow is considered parallel and smooth. With this assumption, the governing equations of motion can be reduced to the form:

\begin{align}
\frac{d^2u}{dz^2} + G\sin\beta &= 0, \\
\frac{dp}{dz} &= -G\cos\beta,
\end{align}

where $u$ is the streamwise velocity component. The boundary conditions are

\begin{equation}
\begin{aligned}
&u(x, 0) = 0, \\
&\frac{\partial u}{\partial z}(x, d) = 0, \\
&p(x, d) = 0,
\end{aligned}
\end{equation}

where $d$ is the thickness of the film. The above equations admit the following solution:

\begin{align}
&u(z) = G\sin\beta \left( dz - \frac{z^2}{2} \right), \\
&w = 0, \\
&p(x, d) = G\cos\beta (d - z).
\end{align}

Equation 2.38 shows that the velocity profile is parabolic where the maximum velocity occurs at the interface, and the pressure is purely hydrostatic. The above solutions are attributed to Nusselt (1916) and hence, known as Nusselt film profile.
In a heated layer, the base state for the temperature field is usually considered as conductive:

$$\theta = 1 - z. \quad (2.41)$$

As discussed in the previous section, the linear analysis using hydrodynamic principles can be applied only in the Region I to study the stability of the ensuing flow. In the classical sense, it is done by perturbing the base flow with a disturbance and analyzing its growth or decay in a spatially or a temporally periodic domain. It is assumed that all the physical properties except the surface tension are constant. The surface tension is taken to depend on the temperature linearly. In addition, the effects of compressibility and the viscous dissipation are neglected. Define nondimensional velocity, pressure and temperature as:

\[
\begin{align*}
\bar{u}(z) + u'(x, y, z, t), \\
v = v'(x, y, z, t), \\
w = w'(x, y, z, t), \\
p = \bar{p}(z) + p'(x, y, z, t), \\
\theta = \bar{\theta}(z) + \theta'(x, y, z, t),
\end{align*}
\]  \quad (2.42)

where the bar denotes the base flow quantity and the prime denotes the perturbation quantity.

\[
\bar{u}(z) = \frac{G \sin \beta}{2} (1 - z^2), \quad (2.43)
\]

\[
\bar{p}(z) = -G \cos \beta z, \quad (2.44)
\]

\[
\bar{\theta}(z) = z. \quad (2.45)
\]
Here, for convenience, we assume that the interface is located at \( z = 0 \) and the plate at \( z = 1 \). With these scaling, the linearized continuity, momentum and the energy equations can be written as:

\[
\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w'}{\partial z} = 0,
\]

\[
\frac{\partial u'}{\partial t} + u \frac{\partial u'}{\partial x} + w \frac{\partial u'}{\partial z} = -\frac{\partial p'}{\partial x} + \left( \frac{\partial^2 u'}{\partial x^2} + \frac{\partial^2 u'}{\partial y^2} + \frac{\partial^2 u'}{\partial z^2} \right),
\]

\[
\frac{\partial v'}{\partial t} + u \frac{\partial v'}{\partial x} = -\frac{\partial p'}{\partial y} + \left( \frac{\partial^2 v'}{\partial x^2} + \frac{\partial^2 v'}{\partial y^2} + \frac{\partial^2 v'}{\partial z^2} \right),
\]

\[
\frac{\partial w'}{\partial t} + u \frac{\partial w'}{\partial x} = -\frac{\partial p'}{\partial z} + \left( \frac{\partial^2 w'}{\partial x^2} + \frac{\partial^2 w'}{\partial y^2} + \frac{\partial^2 w'}{\partial z^2} \right),
\]

\[
\frac{\partial \theta'}{\partial t} + u \frac{\partial \theta'}{\partial x} = \frac{1}{P} \left( \frac{\partial^2 \theta'}{\partial x^2} + \frac{\partial^2 \theta'}{\partial y^2} + \frac{\partial^2 \theta'}{\partial z^2} \right).
\]

To solve these equations, we have to specify the boundary conditions. At the wall, no-slip and constant-temperature conditions are used.

\[
u'(x, y, 1, t) = v'(x, y, 1, t) = w'(x, y, 1, t) = \theta'(x, y, 1, t) = 0.
\]

At the free surface, the normal- and shear-stress conditions, the heat balance, and the kinematic boundary condition are applied. In that process, it is assumed that the slope of the interface is very small and can be neglected, i.e., \( \partial h/\partial x = \partial h/\partial y = 0 \).

\[-\bar{p} - p' + 2 \frac{\partial w'}{\partial z} + 2 \frac{\partial w'}{\partial z} = 6HS,
\]

\[
\frac{\partial \bar{u}}{\partial z} + \frac{\partial u'}{\partial z} + \frac{\partial w'}{\partial x} = \frac{2M}{P} \left( \frac{\partial \theta'}{\partial x} \right),
\]

\[
\frac{\partial v'}{\partial z} + \frac{\partial w'}{\partial y} = \frac{2M}{P} \left( \frac{\partial \theta'}{\partial y} \right),
\]
\[ Bi(\bar{\theta} + \theta') - \frac{\partial \bar{\theta}}{\partial z} - \frac{\partial \theta'}{\partial z} = 0. \]  

(2.55)

Since the interface is perturbed from its equilibrium position by a small quantity \( \eta \), the interfacial conditions shown in Eqs. 2.52 to 2.55 are valid at \( z = \eta \). Hence, we use a Taylor series expansion of the above equations, linearize them, and use them as boundary conditions at \( z = 0 \). We get:

\[-p' - \eta G \cos \beta D\bar{p} + 2 \frac{\partial w'}{\partial z} + 3S \left( \frac{\partial^2 \eta}{\partial x^2} + \frac{\partial^2 \eta}{\partial y^2} \right) = 0, \]  

(2.56)

\[ \eta D^2 \bar{u} + \frac{\partial u'}{\partial z} + \frac{\partial \eta}{\partial x} = \frac{2M}{P} \frac{\partial^2 \theta'}{\partial x \partial z}, \]  

(2.57)

\[ \frac{\partial v'}{\partial z} + \frac{\partial \eta}{\partial y} = \frac{2M}{P} \frac{\partial^2 \theta'}{\partial y \partial z}, \]  

(2.58)

\[ D\theta' = Bi \left( \eta D\bar{\theta} + \theta' \right), \]  

(2.59)

\[ \frac{\partial \eta}{\partial t} + \bar{u} \frac{\partial \eta}{\partial x} = w'. \]  

(2.60)

Substituting the following expressions for the perturbation quantities,

\[
\begin{align*}
    u' &= \bar{u}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right], \\
v' &= \bar{v}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right], \\
w' &= \bar{w}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right], \\
p' &= \bar{p}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right], \\
\theta' &= \bar{\theta}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right], \\
\eta &= \bar{\eta}(z) \exp \left[ i(k_x x + k_y y - \omega t) \right],
\end{align*}
\]  

(2.61)

where \( k_x \) and \( k_y \) are the wavenumbers in the \( x \)- and \( y \)-directions, respectively, and \( \omega \) is the growth rate, the governing equations become:

\[ i \left( k_x \bar{u} + k_y \bar{v} \right) D\bar{w} = 0, \]  

(2.62)
\[ \left\{ D^2 - \left( k_x^2 + k_y^2 \right) - i(k_x \bar{u} - \omega) \right\} \bar{u} = D(\bar{u})\bar{\omega} + i k_x \hat{\rho}, \]  
\text{(2.63)}

\[ \left\{ D^2 - \left( k_x^2 + k_y^2 \right) - i(k_x \bar{u} - \omega) \right\} \bar{v} = i k_y \hat{\rho}, \]  
\text{(2.64)}

\[ \left\{ D^2 - \left( k_x^2 + k_y^2 \right) - i(k_x \bar{u} - \omega) \right\} \bar{\omega} = D(\hat{\rho}), \]  
\text{(2.65)}

\[ \left\{ D^2 - \left( k_x^2 + k_y^2 \right) - i(k_x \bar{u} - \omega) \right\} \bar{\theta} = \bar{\omega}D\bar{\theta}. \]  
\text{(2.66)}

Although the sum of the orders of the equations, Eqs. 2.62 to 2.66, is seven, it is possible to rewrite them into a system of six differential equations of first order (Lin, 1955). However, a remarkable simplification to the above problem can be achieved by using Squire theorem (1933) which states that for any unstable three-dimensional disturbance, there is a corresponding two-dimensional disturbance that is more unstable. This can be obtained by setting \( k_y = 0 \). Then the Eqs. 2.62 to 2.66 reduce to two differential equations, one for \( \bar{\omega}(y) \) and another one for \( \bar{\theta}(y) \):

\[ \left( D^2 - k^2 \right)^2 \bar{\omega} + i \left[ (\omega - k_x \bar{u}) \left( D^2 - k^2 \right) + k_x D^2 \bar{u} \right] \bar{\omega} = 0, \]  
\text{(2.67)}

\[ \left( D^2 - k^2 \right) \bar{\theta} + iP \left[ (\omega - k_x \bar{u}) \bar{\theta} + i \bar{\omega}D\bar{\theta} \right] = 0, \]  
\text{(2.68)}

where,

\[ k = \left( k_x^2 + k_y^2 \right)^{\frac{1}{2}}. \]  
\text{(2.69)}

Equations 2.67 and 2.68 are called as Orr-Sommerfeld equations. The boundary conditions become:

\[ \bar{\omega}(1) = D\bar{\omega}(1) = \bar{\theta}(1) = 0, \]  
\text{(2.70)}

\[ k^2 \left[ G \cos \beta + 3S \right] \hat{\eta} + \left( D^3 - 3k^2 \right) \hat{\omega} + i \left[ \omega - k_x \frac{G}{2} \sin \beta \bar{u}(1) \right] D\hat{\omega}(0) = 0, \]  
\text{(2.71)}
\[
\left( D^2 + k^2 \right) \tilde{w}(0) - k^2 \frac{2M}{P} \tilde{\eta} \tilde{D} \tilde{\theta}(0) - i k_x \tilde{\eta} \tilde{D}^2 \tilde{u}(0) = 0, \quad (2.72)
\]

\[
D \tilde{\theta}(0) = Bi \left( \tilde{\eta} \tilde{D} \tilde{\theta}(0) + \tilde{\theta}(0) \right), \quad (2.73)
\]

where,

\[
\tilde{\eta} = \frac{i \tilde{\omega}}{\left( \omega - k_x \tilde{u} \right)}. \quad (2.74)
\]

The above equation can not be solved analytically and a numerical method has to be employed. In the analysis, the disturbance is considered in the form of a Fourier sum and the response of the system to individual harmonics will decide the stability. For a stable layer, the growth of all the harmonics should decay. Even if there exists a single harmonic for which the system is unstable, the whole system is considered unstable.

In the formulation, \( k \) is the nondimensional wavenumber and \( c = \omega/k \) is the nondimensional phase speed. If \( k \) is fixed strictly real, and \( c \) allowed to be complex, the analysis is called temporal analysis. The disturbance in this case is periodic in space. If the imaginary part of \( c \) is positive, the solution increases exponentially with time and the flow is unstable with respect to that particular mode. If it is negative, this particular mode of disturbance will eventually be damped out and the flow is stable with respect to that particular mode. If \( c \) is fixed real, and \( k \) allowed to take complex values, the analysis is called spatial analysis. The disturbance in this case is periodic in time and its growth in space depends on the sign of the imaginary part of \( k \).

In thin-film flows, there are numerous studies where the temporal-stability analysis has been done by solving the Orr-Sommerfeld equations. Yih (1955, 1963) and Benjamin (1957) first formulated the interfacial-instability problem for an isother-
mal layer. Using small-wavenumber and small Reynolds number approximation, they provided a cut-off $Re$ for the onset of instability:

$$G_c \sin \beta = \frac{5}{2} \cot \beta. \quad (2.75)$$

Equation 2.75 suggests that the flow is always stable in a horizontal layer and is always unstable in a vertical layer. The experimental verification for the above criterion is provided by Liu, Paul & Gollub (1993). The instability in a heated layer was first examined by Pearson (1958) who neglected the surface deformation and the buoyancy effects. Later on, Scriven & Sterling (1964) extended the analysis by considering the surface deformation. They showed that a heated layer is always unstable to long surface waves, and the disturbance of small wavelength exhibits Pearson (1958) type instability. Smith (1966) concluded that gravity becomes important at small wavenumbers and in highly viscous fluid. An extensive analysis of heated layers under the influence of surface-wave and thermocapillary instabilities has been done by Goussis & Kelly (1990, 1991). They reckoned two modes of thermocapillary instability. The first mode is associated with the interaction between the basic temperature field and the velocity perturbation, and manifests itself in the form of convective rolls as first identified by Pearson (1958). This mode occurs either in relatively thick layers or at high intensity of heating,

$$\frac{M}{Bi} > 16.04, \quad (2.76)$$

and the free-surface deformation is not required. The other mode is associated with the variation of the basic temperature with the surface deformation as identified by Scriven & Sterling (1964). This mode occurs in very thin layers if

$$\frac{BiM}{P(1+Bi)^2} > \frac{G}{3} \quad (2.77)$$
and gives rise to severe surface deformation, often resulting in dry spots via rupture process.

2.6 Nonlinear Analysis

The linear stability analysis discussed in the previous section is valid only near the wave-inception region. Beyond this region, the waves grow rapidly so that the nonlinear effects cannot be neglected. In a thin-liquid layer, the disturbances always occur in the form of long surface waves. Since the cut-off wavenumber is very small, most of the nonlinear analyses are done using a small-wavenumber assumption at low Reynolds number. The popular schemes are long-wave evolution equation based on the lubrication theory and boundary-layer type equation based on the boundary-layer approximation. They are briefly discussed next.

2.6.1 Long-Wave Evolution Equation

Small wavenumber expansion based on the lubrication type approximation is the basis for formulating long-wave evolution equation. The approach is to replace the governing equations with a single evolution equation for the interface that is usually a nonlinear partial differential equation. The advantage of using the simplified equation is two fold: the stability of the system can be examined by performing a linear analysis, and the nonlinear dynamics of the flow can be studied by integration. Also, this equation is simpler to solve than the full system of governing equations. However, it is appropriate only when the inertial effects are very small (Joo & Davis, 1992) and fail near spontaneous rupture (Krishnamoorthy, Ramaswamy & Joo, 1995).

(1970), Pumir, Manneville & Pomeau (1983), and Joo, Davis & Bankoff (1991), among others, extended the analysis, included various physical mechanisms, and studied the dynamics of the flow. The early works are summarized by Lin (1983) and more recently by Chang (1994). The derivation of the evolution equation for a two-dimensional heated layer is shown next.

Let $l_c$ be the characteristic length in the $x$-direction that is typically proportional to the wavelength of the disturbance. Using Benney's (1966) expansion for small wavenumber $\epsilon = d/l_c$, we rescale the governing equations and the boundary conditions by introducing,

$$\xi = \epsilon x, \quad \zeta = z, \quad \tau = \epsilon t,$$

(2.78)

where $d$ is the thickness of the layer. Following Joo, et.al. (1991), the scales for the nondimensional parameters are assumed as:

$$G \sim O(1); \quad S = \epsilon^{-2}; \quad \frac{BiM}{P} \sim O(1).$$

(2.79)

The dependent variables are expanded for small $\epsilon$ as:

$$\begin{align*}
    u &= u_0 + \epsilon u_1 + \epsilon^2 u_2 + \cdots, \\
    w &= \epsilon (w_0 + \epsilon w_1 + \epsilon^2 w_2 + \cdots), \\
    p &= p_0 + \epsilon p_1 + \epsilon^2 p_2 + \cdots, \\
    \theta &= \theta_0 + \epsilon \theta_1 + \epsilon^2 \theta_2 + \cdots.
\end{align*}$$

(2.80)

The above equations are substituted back into the rescaled governing equations and the boundary conditions. After rearranging and grouping the terms of equal order in $\epsilon$, a solution for the independent variables is obtained as:
\begin{align*}
\begin{aligned}
u(\xi, \zeta, \tau) &= G(h\xi - \frac{1}{2} \zeta^2) \sin \beta + \frac{2M}{P} \left[ \frac{Bi h}{(1 + Bi h)} \right] \frac{\zeta}{\xi} + \\
&\quad \epsilon \left\{ (Gh_{\xi} \cos \beta - 3\overline{S}h_{\xi\xi\xi\xi}) \left( \frac{1}{2} \zeta^2 - h\zeta \right) + \frac{1}{2} Gh_{\tau} \left( \frac{1}{2} \zeta^3 - h^2 \zeta \right) \sin \beta + \\
&\quad \frac{1}{6} Gh h_{\xi} \left( \frac{1}{4} \zeta^4 - h^3 \zeta \right) \sin^2 \beta + \frac{2M}{P} \left( \frac{Bi h}{1 + Bi h} \right) \frac{\zeta}{\xi} \right\} , \quad (2.81)
\end{aligned}
\end{align*}

\begin{align*}
\begin{aligned}
w(\xi, \zeta, \tau) &= -\epsilon G \sin \beta h_{\xi} \frac{\zeta^2}{2} - \epsilon \frac{M}{P} \left[ \frac{Bi h}{(1 + Bi h)^2} \right] \frac{\zeta^2}{\xi \xi} + \\
&\quad \epsilon^2 \left\{ -G \cos \beta \left( \frac{\zeta^3}{6} h_{\xi\xi} - \frac{\zeta^2}{2} h h_{\xi\xi\xi} - \frac{\zeta^2}{2} h_{\xi} \xi \right) + \\
&\quad 3\overline{S} \left( \frac{\zeta^3}{6} h_{\xi\xi\xi\xi} - \frac{\zeta^2}{2} h h_{\xi\xi\xi\xi} - \frac{\zeta^2}{2} h h_{\xi\xi\xi} \right) - \\
&\quad \frac{G}{2} \sin \beta \left( \frac{\zeta^4}{12} h_{\zeta\zeta} - \frac{\zeta^2}{2} h^2 h_{\zeta\zeta} - \zeta^2 h h_{\xi\zeta} \right) - \\
&\quad \frac{G^2}{6} \sin^2 \beta \left( \frac{\zeta^5}{20} h^2 - 2\zeta^2 h^3 h_{\xi\zeta} + \frac{\zeta^5}{20} h h_{\xi\xi} - \frac{\zeta^2}{2} h^4 h_{\xi\xi} \right) \right\} , \quad (2.82)
\end{aligned}
\end{align*}

\begin{align*}
p &= G \left( h - \zeta \right) \cos \beta - 3\overline{S} h_{\xi\xi} + \epsilon \{ \cdots \}, \quad (2.83)
\end{align*}

and

\begin{align*}
T &= 1 - \left[ \frac{\zeta Bi}{1 + Bi h} \right] + \epsilon \{ \cdots \}. \quad (2.84)
\end{align*}

In the above expressions, the leading order pressure \(p_0\) is composed of the hydrostatic pressure and the capillary effects, and the leading order heat transfer is purely conductive. However, these can be modified by the second order unsteady and convective effects. Equations 2.81 to 2.84 are substituted into the kinematic condition to obtain the evolution equation for the film thickness \(h(\xi, \tau)\). When rescaled back, the final form of the equation is expressed as:
\begin{align*}
&h_t + G h^3 h_x \sin \beta + \left( \frac{2G^2}{15} h^5 h_x \sin^2 \beta \\
&+ \frac{BiM}{P} \left[ \frac{h^2 h_x}{(1 + Bi h)^2} \right] - \frac{G}{3} h^3 h_x \cos \beta + Sh^3 h_{xxx} \right)_{x} + O(\epsilon^2) = 0. \tag{2.85}
\end{align*}

In the above equation, the second term describes the wave propagation, while the third term describes the mean shear flow. The fourth, fifth and the sixth terms describe the thermocapillarity, the hydrostatic effect and the mean surface tension, respectively. Further simplification to the above equation is possible by carrying out an expansion for a small amplitude \( \eta \), where \( h=1+\eta \). In the limit \( S \to \infty \), the expansion yields an equation for a one-dimensional wave without \( z \) variation, known as Kuramoto-Sivashinsky (KS) equation (Lin, 1974; Nepomnyashy, 1974):

\begin{align*}
\eta_t + a \eta \eta_x + b \eta_{xx} + c \eta_{xxx} + O(\eta^2) = 0, \tag{2.86}
\end{align*}

where \( a, b, \) and \( c \) are the appropriate constants. The above equation is written for a vertically falling film. The KS equation is more restrictive than the long-wave evolution equation because of the additional stipulation that the deviation in the amplitude \( (\eta) \) must be small. In a typical thin-film flow, it is possible to have a situation where the amplitude of the wave is very small when compared to the wavelength and still be the same order of magnitude as the Nusselt film thickness.

Both the long-wave evolution and KS equations are very popular among many research scholars due to their relative simplicity. However, these equations are valid only for fluids with strong surface tension unless the higher order terms are included in their formulation. They fail to follow the dynamics when the flow becomes highly nonlinear.
2.6.2 Boundary-Layer Approximation

As the film thickness increases, $G \gg 1$, the inertial effects become significant and the long-wave evolution and the KS equations are not useful to study the dynamics. Hence, instead of lubrication theory, it will be appropriate to use a boundary-layer type approximation. This was first studied by Shkadov, Kholpanov, Malyusov & Zhavoronkov (1970). For a two-dimensional isothermal flow, the boundary-layer equations are:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} = G\sin\beta - G\cos\beta h_x + 3S \frac{\partial^3 h}{\partial x^3} + \frac{\partial^2 u}{\partial z^2},
\]

\[
\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0,
\]

where the diffusion term in the streamwise ($x$) direction is assumed very small and is neglected. For a two-dimensional wave, the above equations can be further simplified using an integral boundary-layer theory (Chang, 1994). This can be done by assuming a self-similar parabolic profile for the flow. One obtains:

\[
\frac{\partial Q}{\partial t} + \frac{6}{5} \frac{\partial}{\partial x} \left( \frac{Q^2}{h} \right) = h \left[ G\sin\beta - G\cos\beta h_x + 3S \frac{\partial}{\partial x} \left( \frac{1}{R} \right) \right] - \frac{3Q}{h^2},
\]

\[
\frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} = 0,
\]

where

\[
Q = \int_0^{h(x,t)} u \, dz,
\]

is the volumetric flow rate per unit span width. Further, the above two equations (Eqs. 2.89 and 2.90) can be collapsed into a single second-order wave equation for the film thickness $h(x,t)$ (Alekseenko, Nakoryakov & Pokusaev, 1985). Extensive nonlinear studies using the numerical simulation of the boundary-layer approximation have been done by Chang, Demekhin & Kopelevich (1993). A more recent
review on this method can be found in Chang (1994). Although the boundary-layer approximation is valid for high Reynolds number flows, it still uses the assumption that the disturbances appear in the form of long surface waves. Hence, to study the thin-film flow dynamics thoroughly, one should use the full-scale computation.

2.7 Numerical Studies

Several numerical simulations of thin-film flows have been done in the past two decades. They can be classified into two types: simulation of simplified equations and the simulation of the full-system of the governing equations. As explained in the previous section, all the model equations possess disadvantages based on the type of approximation used in their formulation. They become invalid when the inertia of the mean flow is very significant. This situation can arise near wave breaking or near rupture. Hence, a complete system of governing equations coupled with fully-nonlinear boundary conditions needs to be solved.

Most of the direct numerical simulation of thin-film flows are focused on isothermal layers (Bach & Villadsen, 1984; Khashgi & Scriven, 1987; Ho & Patera 1990; Malamataris & Papanastasiou 1991; Salamon, Armstrong & Brown, 1994; Chippada, Ramaswamy & Joo, 1996). To author's knowledge, the literature available in non-isothermal film flows is scarce. Due to the irregular and the time-varying computation domain involved, the finite-element method has been a popular choice of numerical scheme. Bach & Villadsen (1984), Khashgi & Scriven (1987) and Malamataris & Papanastasiou (1991) use a Lagrangian finite-element Method to handle moving boundary and control mesh distortion through rezoning. Khashgi & Scriven (1987) used Galerkin weighted residual, implicit predictor corrector, mixed finite-element formulation and studied isothermal thin-film flows. Ho & Patera (1990) studied the stability of these flows using the Legendre spectral-element method. They made
comparisons with Orr-Sommerfeld theory and the experimental work of Kapitza & Kapitza (1949) to validate the numerical scheme. Salamon, et. al. (1994) solved finite-element equations written in a reference frame translating at wave speed to study specifically the finite-amplitude saturated waves. They found good agreement with the long-wave theory for small-amplitude waves, but found their results to qualitatively diverge for large-amplitude waves. They also studied the nonlinear interaction between the waves and the secondary subharmonics bifurcation to longer waves.

Krishnamoorthy, et. al. (1995), solved the governing equations written in Arbitrary Lagrangian Eulerian frame of reference and showed that when the interfacial mode of thermocapillarity is dominant, all horizontal layers will eventually rupture. Recently, Chippada, et. al. (1996) solved the full system of governing equations and studied various nonlinear phenomena in an isothermal layer. They provided, for the first time, a nonlinear phase diagram that shows the phase boundary for the quasiperiodic flow behavior. They also verified various experimental studies through direct numerical simulation.
Chapter 3

Numerical Scheme

3.1 Introduction

Thin-film flow problems involve a comprehensive analysis of the local-flow pattern and require accurate tracking of the interface. At every time level, the governing equations must be solved accurately, in a geometrically deforming computational domain, to study the temporal evolution of the flow. To facilitate these tedious calculations, we choose to solve the system of equations in an Arbitrary Eulerian Lagrangian (ALE) frame of reference using a finite-element method (FEM) based on a projection scheme.

There are two ways of solving the system based on the method of formulating the governing equations: the primitive variable formulation and the stream function-vorticity formulation. In the primitive variable formulation, the governing equations are solved directly for the unknown variables $u$, $v$, $w$, $p$ and $\theta$. The advantage of using this method is that the boundary conditions can be incorporated naturally and easily. However, the time-stepping procedure for pressure is not straightforward, since, the time derivative for the pressure does not appear explicitly in the momentum equations. In the stream function-vorticity formulation, the governing equations are written in terms of the stream function and the vorticity by taking the curl of the momentum equations. This procedure eliminates the pressure and satisfies the continuity constraint automatically. However, prescribing the boundary conditions particularly for the pressure and the vorticity becomes very difficult. In
a free-surface flow problem, the pressure always appears as a boundary condition due to the normal stress condition, and hence, we choose to solve the problem in the primitive variable form.

In a moving-boundary problem, the flow domain has an unknown boundary that has to be calculated as a part of the solution procedure. Some specific examples are the problems that involve a phase-change, propagation of flames, draining liquid layers and various other applications where the interfacial phenomenon is significant. This problem is highly nonlinear and an analytical solution is extremely difficult to obtain. Hence, numerical methods are widely used. There are two approaches to modeling the interface (Floryan & Rasmussen, 1989): the interface capturing methods and the interface tracking methods. In a capturing method, the interface is resolved by calculating the sharply varying fluid properties near its vicinity and no special model is used. In a tracking method, the interface is treated as a discontinuity in the flow domain and a suitable model is used to locate the interface explicitly. In this dissertation, a tracking algorithm that uses the kinematic condition to update the free surface is used.

The interface-tracking algorithms can be further classified into three different categories depending on the frame of reference used in the calculation (Floryan & Rasmussen, 1989): an Eulerian, a Lagrangian, and a mixed Eulerian Lagrangian. In an Eulerian method, the governing equations are solved in a coordinate system that is stationary in the laboratory frame of reference or is moving in a prescribed manner. Here, the fluid particles are allowed to move across the computational cell. Since the interface is not defined sharply, the implementation of free-surface conditions becomes very difficult. Some of the popular methods that fall into this category are the Marker and Cell (MAC) method (Harlow & Welsch, 1966) and the Volume Of Fluid (VOF) method (Hirt & Nichols, 1981). In a Lagrangian method, the governing
equations are solved in a coordinate system that moves with the fluid particles. A group of methods called particle methods also fall into this category. Here, the fluid particles are not allowed to move across the cell and each cell always contains the same fluid element. Though this method defines the interface sharply, the mesh tangling and distortion can happen and lead to loss of information and inaccurate solutions. A popular method in this category is Lagrangian Incompressible (LINC) method developed by Hirt, Cook & Butler (1970). In a mixed Eulerian Lagrangian method, the governing equations are written in a reference coordinate system that moves independent of the fluid particles. This method combines the advantage of both Eulerian and Lagrangian methods without their disadvantage such as mesh distortion. The full interfacial conditions can be implemented and the interface can be tracked accurately. A popular method in this category is the arbitrary Eulerian Lagrangian (ALE) formulation proposed by Hirt, Amsden & Cook (1974). The present work also uses ALE formulation which is explained in the Sect. 3.2.

In Sect. 3.3, the time-stepping procedure is discussed in detail. In Sect. 3.4, spatial discretization using the Galerkin-Bubnov method is explained. Some issues in the free-surface modeling, specific to the present study, are addressed in Sect. 3.5.

3.2 ALE Formulation

Here, the governing equations are written in a frame of reference that moves independent of the fluid motion. This formulation was proposed initially by Hirt, Amsden & Cook (1974) and later on used by many researchers (Chan, 1975; Hughes, Liu & Zimmerman 1981; Ramaswamy & Kawahara 1987; Ramaswamy, 1990; Soulaimani, Fortin, Dhatt & Ouellet, 1991; Chippada et al., 1996; Chippada, 1995; Chippada, Jue & Ramaswamy, 1995) in modeling free-surface flow problems and fluid-structure
interaction problems (Donea, Giuliani & Halleux, 1982; Donea, 1983; Liu, Chang, Chen & Belytschko, 1988). ALE formulation has been derived by Donea et al. (1982), Ramaswamy & Kawahara (1987), Soulaimani et al. (1991), Lacroix & Garon (1992), among many others and is briefly described next (Chippada 1995).

Let $B_0$ be the open region occupied by fluid particles at $t=0$ as shown in Fig. 3.1. This is also called material domain. The position vector of a point $P$ in $B_0$ is denoted by $X_i=(X_1,X_2,X_3)$. $B_t$ is the open region occupied by $B_0$ after some time $t>0$. The point $P$ occupies a unique point $p$ in $B_t$ whose position vector is denoted by $x_i=(x_1,x_2,x_3)$. It is assumed that the mapping between $P$ and $p$ is continuous, unique and invertible.

$$x_i = \phi(X_i,t) \quad X_i = \phi^{-1}(x_i,t) \quad \text{(3.1)}$$

The Lagrangian (material) velocity is defined as

$$\dot{x}_i(X_i,t) = \frac{\partial}{\partial t} \phi(X_i,t) \quad \text{(3.2)}$$

and the Lagrangian acceleration is defined as

$$\ddot{x}_i(X_i,t) = \frac{\partial^2}{\partial t^2} \phi(X_i,t) \quad \text{(3.3)}$$

In terms of spatial coordinate $x_i$, the Eulerian velocity is defined as

$$u_i(x_i,t) = \frac{\partial}{\partial t} \phi(x_i,t) \quad \text{(3.4)}$$

and the Eulerian acceleration can be shown to take the form:

$$a_i(x_i,t) = u_{i,t}(x_i,t) + u_j(x_i,t)u_{i,j}(x_i,t) \quad \text{(3.5)}$$

where nonlinear convective terms appear.

In the ALE formulation, a third domain called the referential domain is specified. At time $t=0$, it occupies an open region $R_0$. This domain has its own motion and at some time later, $t>0$, it coincides with the material domain that has moved to
Figure 3.1: Arbitrary Lagrangian Eulerian description of the flow. Figure adopted from Chippada (1995).

$B_t$. That is, the referential point $q$ whose position vector is $\hat{x}_i=(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ coincides with point $p$ in space coordinate after some time $t>0$. The mapping between these two regions is given by

$$x_i = \lambda(\hat{x}_i, t)$$ (3.6)

and the referential velocity ($\hat{g}_i$) will be

$$\hat{g}_i(x_i, t) = \frac{\partial}{\partial t} \lambda(\hat{x}_i, t)$$ (3.7)

The relative motion of the fluid with respect to the referential frame is expressed as

$$\hat{x}_i = \lambda^{-1}(x_i, t) = \lambda^{-1}(\phi(X_i, t), t) = \psi(X_i, t)$$ (3.8)

and the relative velocity is
\[ \hat{V}_i^\psi(\hat{x}_i, t) = \frac{\partial}{\partial t} \psi(X_i, t) \bigg|_{X_i} \]  
(3.9)

The material point \( P \) and the referential point \( q \) arrive at the spatial point \( p \) through independent motions that are related as follows:

\[ x_i = \lambda(\hat{x}_i, t) = \lambda(\psi(X_i, t), t) = \phi(X_i, t) \]  
(3.10)

From the above relation, we can derive

\[ u_i(x_i, t) = \hat{u}_i(\hat{x}_i, t) = \frac{\partial}{\partial t} \lambda(\psi(X_i, t), t) \bigg|_{X_i} \]  
(3.11)

\[ = \frac{\partial \lambda}{\partial t}(\hat{x}_i, t) + \hat{F}_{ij}(\hat{x}_i, t) \hat{V}_i^\psi(\hat{x}_i, t) \]  
(3.12)

\[ = \hat{g}_i(\hat{x}_i, t) + \hat{F}_{ij}(\hat{x}_i, t) \hat{V}_i^\psi(\hat{x}_i, t) \]  
(3.13)

where, \( \hat{F}_{ij} \) is called gradient deformation tensor defined as

\[ \hat{F}_{ij}(\hat{x}_i, t) = \frac{\partial x_i}{\partial \hat{x}_j} \]  
(3.14)

The spatial acceleration in the referential coordinates can be shown to be:

\[ a_i(x_i, t) = \hat{u}_{i,t} + \hat{V}_i^\psi \hat{u}_{i,j}(\hat{x}_i, t) \]  
(3.15)

\[ = \hat{u}_{i,t} + \hat{F}_{ij}^{-1}(\hat{u}_j - \hat{g}_j) \hat{u}_{i,j}(\hat{x}_i, t) \]  
(3.16)

Comparing spatial acceleration (Eq. 3.5) with referential acceleration (Eq. 3.16), the difference is that gradients are with respect to referential coordinate, and the spatial velocity is replaced by the relative velocity. Equation 3.16 can also be interpreted as a statement of the material conservation laws with respect to arbitrary moving points. In the event a grid point coincides with the material point, the relative velocity \( (\hat{V}_i^\psi(\hat{x}_i, t)) \) becomes zero. Consequently, the set of equations becomes Lagrangian. Similarly, a pure Eulerian description can be obtained by setting \( \hat{g}_i \) to zero. The ALE approach combines both Lagrangian and Eulerian methods. In our problem, the referential motion is related to the fluid motion, and at the free boundary, the mesh points are moved normal to the interface with fluid velocity to
prevent the loss or gain of fluid material. In our problem, the referential motion is related to the fluid motion and at the free boundary, the mesh points are moved normal to the interface with the fluid velocity to prevent the loss or gain of fluid material. With this simplification, we rewrite the governing equations as:

Conservation of mass:
\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad (3.17)
\]

Conservation of momentum:
\[
\begin{align*}
\frac{\partial u}{\partial t} &+ (u - g_x)\frac{\partial u}{\partial x} + (v - g_y)\frac{\partial u}{\partial y} + (w - g_z)\frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + G\sin\beta + \\
&\quad \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right),
\end{align*}
\]
\[
\left\{ (3.18)
\right. 
\]
\[
\begin{align*}
\frac{\partial v}{\partial t} &+ (u - g_x)\frac{\partial v}{\partial x} + (v - g_y)\frac{\partial v}{\partial y} + (w - g_z)\frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \\
&\quad \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right),
\end{align*}
\]
\[
\left(3.19\right)
\]
\[
\begin{align*}
\frac{\partial w}{\partial t} &+ (u - g_x)\frac{\partial w}{\partial x} + (v - g_y)\frac{\partial w}{\partial y} + (w - g_z)\frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} - G\cos\beta + \\
&\quad \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right),
\end{align*}
\]
\[
\left. (3.20) \right.
\]

Conservation of energy:
\[
\frac{\partial \theta}{\partial t} + (u - g_x)\frac{\partial \theta}{\partial x} + (v - g_y)\frac{\partial \theta}{\partial y} + (w - g_z)\frac{\partial \theta}{\partial z} = \\
\quad \frac{1}{P} \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2} \right), \quad (3.21)
\]

where \( g_x, g_y, \) and \( g_z \) are respectively, the grid-point velocities in \( x, y, \) and \( z \) directions.
3.3 Fractional Step Method

The governing equations, along with the boundary conditions, are integrated in the primitive form to compute the unknown variables $u$, $v$, $w$, $p$ and $\theta$ using a semi implicit/explicit finite-element method. In this scheme, the advective terms are integrated explicitly, while the diffusive terms are integrated implicitly. The projection method, proposed initially by Chorin (1968) in finite difference context and based on Helmholtz decomposition theorem, is employed. The highlights of the scheme are: decoupling the pressure from the momentum equations; solving a pressure Poisson equation; and using a velocity correction procedure to satisfy the incompressibility constraint. The splitting of the velocity components from the pressure admits the implementation of a fast iterative solver and thus, reduces computational time and storage significantly.

From the previous time step ($n$) velocity $(u^n, v^n, w^n)$, pressure $(p^n)$, and temperature $(\theta^n)$, the respective new time level ($n+1$) values $(u^{n+1}, v^{n+1}, w^{n+1}, p^{n+1}$, and $\theta^{n+1}$) are calculated as follows:

**Step 1**: An intermediate velocity field $(\tilde{u}^{n+1}, \tilde{v}^{n+1}, \tilde{w}^{n+1})$ is calculated by omitting the pressure term from the momentum equations. In the present work, this is accomplished by adopting a semi implicit/explicit approach. The nonlinear convective terms are integrated using the second-order Adams-Bashforth explicit method and the diffusive terms are integrated using the first-order Euler's method.

\[
\begin{align*}
\frac{\tilde{u}^{n+1} - u^n}{\Delta t} - \nabla^2 \tilde{u}^{n+1} &= -\frac{3}{2}(u^n - g_x^n) \frac{\partial u^n}{\partial x} + \frac{1}{2}(u^{n-1} - g_x^{n-1}) \frac{\partial u^{n-1}}{\partial x} - \\
&\quad \frac{3}{2}(v^n - g_y^n) \frac{\partial u^n}{\partial y} + \frac{1}{2}(v^{n-1} - g_y^{n-1}) \frac{\partial u^{n-1}}{\partial y} - \\
&\quad \frac{3}{2}(w^n - g_z^n) \frac{\partial u^n}{\partial z} + \frac{1}{2}(w^{n-1} - g_z^{n-1}) \frac{\partial u^{n-1}}{\partial z} + f_x^n.
\end{align*}
\]
\[
\frac{\tilde{u}^{n+1} - u^n}{\Delta t} - \nabla^2 \tilde{u}^{n+1} = \frac{3}{2} (u^n - g_x^n) \frac{\partial v^n}{\partial x} + \frac{1}{2} (u^{n-1} - g_x^{n-1}) \frac{\partial v^{n-1}}{\partial x} - \\
\frac{3}{2} (v^n - g_y^n) \frac{\partial v^n}{\partial y} + \frac{1}{2} (v^{n-1} - g_y^{n-1}) \frac{\partial v^{n-1}}{\partial y} - \\
\frac{3}{2} (w^n - g_z^n) \frac{\partial v^n}{\partial z} + \frac{1}{2} (w^{n-1} - g_z^{n-1}) \frac{\partial v^{n-1}}{\partial z} + f_y^n. \\
\]

(3.23)

\[
\frac{\tilde{w}^{n+1} - w^n}{\Delta t} - \nabla^2 \tilde{w}^{n+1} = \frac{3}{2} (v^n - g_y^n) \frac{\partial w^n}{\partial y} + \frac{1}{2} (v^{n-1} - g_y^{n-1}) \frac{\partial w^{n-1}}{\partial y} - \\
\frac{3}{2} (w^n - g_z^n) \frac{\partial w^n}{\partial z} + \frac{1}{2} (w^{n-1} - g_z^{n-1}) \frac{\partial w^{n-1}}{\partial z} + f_z^n. \\
\]

(3.24)

Here, \(f_x, f_y,\) and \(f_z\) are respectively the components of the load vector arising from the body force term. In this step, the Dirichlet and the Neumann boundary conditions for the velocity components are imposed. Since the pressure term is omitted, the intermediate velocity field need not satisfy the incompressibility constraint.

**Step 2:** In this step, the pressure is calculated from the intermediate velocity field by projecting it on a divergence-free space. This results in a Poisson equation that is solved to calculate \(p^{n+1}.\) The boundary conditions are Neumann condition on the solid walls and the normal-stress condition at the interface.

\[
\nabla^2 p^{n+1} = \frac{1}{\Delta t} \left( \frac{\partial \tilde{u}^{n+1}}{\partial x} + \frac{\partial \tilde{v}^{n+1}}{\partial y} + \frac{\partial \tilde{w}^{n+1}}{\partial z} \right).
\]

(3.25)

**Step 3:** Using the intermediate velocity field and new pressure, we calculate the final velocity field \((u^{n+1}, v^{n+1}, w^{n+1})\) by employing a velocity correction procedure. In this method, suitable contribution of the pressure field is added to \(\tilde{u}^{n+1}, \tilde{v}^{n+1},\) and \(\tilde{w}^{n+1}:\)

\[
\frac{u^{n+1} - \tilde{u}^{n+1}}{\Delta t} = - \frac{\partial p^{n+1}}{\partial x},
\]

(3.26)

\[
\frac{v^{n+1} - \tilde{v}^{n+1}}{\Delta t} = - \frac{\partial p^{n+1}}{\partial y},
\]

(3.27)
\[
\frac{w^{n+1} - \bar{w}^{n+1}}{\Delta t} = -\frac{\partial p^{n+1}}{\partial z}.
\] (3.28)

After the final velocity is calculated, the temperature field is computed. The energy equation is integrated in a single step to obtain final temperature \(\theta^{n+1}\). We use a semi implicit/explicit approach similar to the one discussed in step 1.

\[
\begin{align*}
\frac{\hat{\theta}^{n+1} - \theta^n}{\Delta t} - \nabla^2 \hat{\theta}^{n+1} &= -\frac{3}{2}(u^n - g_x^n)\frac{\partial \theta^n}{\partial x} + \frac{1}{2}(u^{n-1} - g_x^{n-1})\frac{\partial \theta^{n-1}}{\partial x} - \\
&\quad \frac{3}{2}(v^n - g_y^n)\frac{\partial \theta^n}{\partial y} + \frac{1}{2}(v^{n-1} - g_y^{n-1})\frac{\partial \theta^{n-1}}{\partial y} - \\
&\quad \frac{3}{2}(w^n - g_z^n)\frac{\partial \theta^n}{\partial z} + \frac{1}{2}(w^{n-1} - g_z^{n-1})\frac{\partial \theta^{n-1}}{\partial z} + f_\theta^n,
\end{align*}
\] (3.29)

where \(f_\theta\) is the load vector that arises from the body force term.

### 3.4 Spatial Discretization

The spatial discretization of the flow domain is done using a linear-tetrahedral element for the three-dimensional problem and a linear-triangular element for the two-dimensional flow problem. These elements are called linear because the unknown variables \((u, v, w, p, \text{ and } \theta)\) are defined at all the nodes located at the vertices of the element and are interpolated linearly across the element faces. This formulation is also known as equal-order approximation. This can be expressed as:

\[
u^{(i)} = N^{(i)}_\alpha u_\alpha, \quad (3.30)
\]

\[
u^{(i)} = N^{(i)}_\alpha v_\alpha, \quad (3.31)
\]

\[
u^{(i)} = N^{(i)}_\alpha w_\alpha, \quad (3.32)
\]

\[
u^{(i)} = N^{(i)}_\alpha p_\alpha, \quad (3.33)
\]

\[
u^{(i)} = N^{(i)}_\alpha \theta_\alpha, \quad (3.34)
\]
where, $N$ is the shape (interpolation) function, the subscript $\alpha$ denotes the local node of the element ($\alpha=1,2,3$ for a triangular element and $1,2,3,4$ for a tetrahedral element), and the superscript $i$ is the location where the variable is calculated. For an explicit expression for these shape functions refer Chung (1977). We use the Galerkin-Bubnov method, that considers weighting functions same as the interpolation functions, and obtain the following element matrices:

\begin{align}
M_{\alpha\beta}^e &= \int_{\Omega_e} N_\alpha N_\beta \, d\Omega_e, \\
L_{\alpha\beta}^e &= \int_{\Omega_e} N_\alpha,; N_\beta,; \, d\Omega_e, \\
C_{\alpha\beta\gamma i}^e &= \int_{\Omega_e} N_\alpha N_\beta N_\gamma,; \, d\Omega_e, \\
P_{\alpha\beta\gamma i}^e &= \int_{\Omega_e} N_\alpha N_\beta,; N_\gamma,; \, d\Omega_e, \\
F_{ai}^e &= \int_{\Omega_e} N_\alpha f_i \, d\Omega_e,
\end{align}

where $M_{\alpha\beta}^e$, $L_{\alpha\beta}^e$, $C_{\alpha\beta\gamma i}^e$, and $P_{\alpha\beta\gamma i}^e$ are, respectively, the element level Mass, Laplacian or diffusion, convection, and pressure matrices and $F_{ai}^e$ is the body force vector. The superscript $e$ denotes the element and the subscript $i$ represents the differentiation of the shape functions with respect to the $i^{th}$ spatial coordinate ($i=x, y, z$). Note that we have used tensor notation in Eqs. 3.35 to 3.39. The discretized form of the projection scheme can be expressed as:

Step 1: \[
\begin{align*}
\left(M_{\alpha\beta}^e + \Delta t L_{\alpha\beta}^e \right) U_{i\beta}^{n+1} &= M_{\alpha\beta}^e U_{i\beta}^n - \frac{3}{2} C_{\alpha\beta\gamma i}^e (U_{i\beta}^n - G_{i\beta}^n) U_{j\gamma}^n + \\
&\quad \left( \frac{1}{2} C_{\alpha\beta\gamma i}^e (U_{i\beta}^{n-1} - G_{i\beta}^{n-1}) U_{j\gamma}^{n-1} \right) F_{ai}^e,
\end{align*}
\]
where, \( U=(u, v, w) \) is the velocity vector and \( G=(g_x, g_y, g_z) \) is the grid-point velocity vector.

**Step 2:**

\[
L^e_{\alpha\beta} p_{\beta}^{n+1} = P^e_{\alpha\beta} \tilde{U}_{i\beta}. \tag{3.41}
\]

**Step 3:**

\[
M^{L^e}_{\alpha\beta} U^i_{\alpha}^{n+1} = M^{L^e}_{\alpha\beta} U^i_{\beta}^{n} - P^e_{\alpha\beta} p_{\beta}^{n+1}. \tag{3.42}
\]

Here, \( M^{L^e}_{\alpha\beta} \) is the lumped mass matrix in which the elements of each row of the consistent mass matrix \( M^e_{\alpha\beta} \) are summed and placed in the main diagonal.

The element-level equations are assembled into a global matrix. The symmetric property of \( M^e_{\alpha\beta} \) and \( L^e_{\alpha\beta} \) are fully exploited to reduce the computational storage. A conjugate gradient solver is used to solve the linear system of equations.

### 3.5 Free-surface Calculation

The governing equations written in the ALE frame of reference are integrated using the projection method explained in the previous section. In this phase of calculation, the normal-stress condition at the interface is incorporated directly into the momentum equations while the tangential-stress conditions are applied as a natural boundary condition. As explained earlier, our numerical scheme is a tracking method and calculates the free-surface location at every time level after the computation of the primitive variables. We achieve this by solving the conservative form of the kinematic equation;

\[
\frac{\partial h}{\partial t} + \frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} = 0, \tag{3.43}
\]

where,

\[
Q_x = \int_0^{h(x,y,t)} u(x,y,z) \, dz, \tag{3.44}
\]
is the volume flow rate in the $x$-direction, and

$$Q_y = \int_0^{h(x,y,t)} u(x, y, z) \, dz,$$

(3.45)

is the volume flow rate in the $y$-direction. The above equation is integrated in time using the second-order leap-frog scheme and in space using Fourier Spectral Method (FSM). Using $h^{n+1}$, the new location of the grid points and the corresponding grid velocity are calculated. The conservative form is used for the reasons discussed below.

The purpose of this research is to investigate the dynamics of a heated layer draining on an inclined plate. Our study is focused mainly on the temporal stability analysis where the evolution of the layer is investigated on a spatially periodic domain. In the absence of the mean flow, the liquid-air interface will maintain a symmetric shape if the imposed disturbance is symmetric. A specific example is the evolution of a horizontal layer heated from below. In such simulations, we need to accurately calculate the interface shape and hence, a spectral method will be very helpful. It is easier to implement the spectral method in the conservative form rather than in the local-velocity form.

After the free-surface computation, the grid points are distributed using a rezoning technique. In this method, we assume that all the grid points are resting on vertical spines spaced equally along the domain. The nodes are allowed to move only up or down depending on the free-surface location. This is possible due to the ALE formulation used in the numerical scheme. Once the new locations of the grid points are calculated, the grid-point velocity in the $z$ direction is computed as:

$$g_z = \frac{z^{n+1} - z^n}{\Delta t},$$

(3.46)

We do not move the nodes in the streamwise and spanwise directions, $g_x$ and $g_y$ are zero.
Since the diffusion terms are treated implicitly, the restriction on the time step is imposed by the advection terms only. The time step for the integration is chosen such that the CFL (Courant-Friedrichs-Levy) condition is always satisfied;

\[ \Delta t \leq C \min \left( \frac{\Delta x}{|u| + \sqrt{Gh + \frac{3S}{h}}}, \frac{\Delta y}{|v| + \sqrt{Gh + \frac{3S}{h}}}, \frac{\Delta z}{|w|} \right), \]  

(3.47)

where \( C \) is the Courant number and \( C \leq 1 \) for a stable scheme. The terms inside the square root represent the contributions from gravity and capillary waves, respectively. In most of the simulations, a Courant number in the range of 0.1-0.5 is used.

### 3.6 Code Validation

A code has been developed that uses the projection algorithm to solve the governing equations. To validate the code, a two-dimensional benchmark problem suggested by De Vahl Davis & Jones (1983) and De Vahl Davis (1983) is solved, and the solutions compared. Here, a Boussinesque fluid of Prandtl number 0.71 is considered in an upright cavity as shown in Fig. 3.2. The length and height of the cavity are \( D \). All the velocity components are zero on the solid wall. The left wall is maintained at a temperature \( T_1 \) and the right wall at a temperature \( T_2 \) (\( T_2 < T_1 \)). The top and the bottom walls are insulated. Using the nondimensional coordinates; \( x^* = x/D \) and \( z^* = z/D \), the nondimensional velocities; \( u^* = uD/\alpha \) and \( w^* = wD/\alpha \), and the nondimensional temperature \( \theta = ([T-T_2]/[T_1-T_2]) \), we write the governing equations, after dropping * for convenience, as:

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \]  

(3.48)

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + P\nabla^2 u, \]  

(3.49)
Figure 3.2: Physical configuration of the benchmark problem suggested by De Vahl Davis & Jones (1983).

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + P \nabla^2 v + Pr \theta, \tag{3.50}
\]

\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} = \nabla^2 \theta, \tag{3.51}
\]

where, \(\alpha\) is the thermal diffusivity, \(P\) is the Prandtl number \((P = \nu/\alpha)\), \(\nu\) is the kinematic viscosity of the fluid, \(Ra\) is the Rayleigh number,

\[
Ra = \frac{\beta g (T_1 - T_2) D^3}{\nu \alpha}, \tag{3.52}
\]

\(\beta\) is the coefficient of volumetric expansion. The boundary conditions are:

\[
\begin{align*}
   u(x, 0, t) &= w(x, 0, t) = 0, \\
   u(x, 1, t) &= w(x, 1, t) = 0, \\
   u(0, z, t) &= w(0, z, t) = 0, \\
   u(1, z, t) &= w(1, z, t) = 0, \\
\end{align*}
\tag{3.53}
\]
\[
\begin{align*}
\theta(0, z, t) &= 1, \\
\theta(1, z, t) &= 0, \\
\frac{\partial \theta}{\partial z}(x, 0, t) &= 0, \\
\frac{\partial \theta}{\partial z}(x, 1, t) &= 0. \\
\end{align*}
\]

(3.54)

The results from our calculations are presented in Tables 3.1 to 3.4 for \(Ra=10^3, 10^4, 10^5\) and \(10^6\), respectively, and are compared with those of the benchmark solutions. As it is seen, with fine enough mesh the computed solutions agree very well with the benchmark solutions.

The next step is to validate the free-surface calculation. In this regard, we compare the evolution of the interface predicted by the current numerical method with that of the spectral computation of the long-wave evolution equation. As we discussed before, this equation is a simplified model and the comparison of the results during the initial period of evolution is a good way of checking the accuracy of our code. To accomplish this, we represent the shape of the interface as:

<table>
<thead>
<tr>
<th>Property</th>
<th>20x20</th>
<th>% error</th>
<th>40x40</th>
<th>% error</th>
<th>Bench mark</th>
</tr>
</thead>
<tbody>
<tr>
<td>(u_{\text{max}})</td>
<td>3.638</td>
<td>-0.30</td>
<td>3.647</td>
<td>-0.05</td>
<td>3.649</td>
</tr>
<tr>
<td>(y)</td>
<td>0.800</td>
<td>-1.60</td>
<td>0.825</td>
<td>1.50</td>
<td>0.813</td>
</tr>
<tr>
<td>(v_{\text{max}})</td>
<td>3.691</td>
<td>-0.16</td>
<td>3.713</td>
<td>0.43</td>
<td>3.697</td>
</tr>
<tr>
<td>(x)</td>
<td>0.200</td>
<td>1.10</td>
<td>0.175</td>
<td>-1.60</td>
<td>0.178</td>
</tr>
<tr>
<td>(Nu)</td>
<td>1.115</td>
<td>-0.27</td>
<td>1.117</td>
<td>-0.09</td>
<td>1.118</td>
</tr>
<tr>
<td>(Nu_{1/2})</td>
<td>1.115</td>
<td>-0.27</td>
<td>1.118</td>
<td>0.00</td>
<td>1.118</td>
</tr>
<tr>
<td>(Nu_0)</td>
<td>1.113</td>
<td>-0.36</td>
<td>1.117</td>
<td>0.00</td>
<td>1.117</td>
</tr>
<tr>
<td>(Nu_{\text{max}})</td>
<td>1.494</td>
<td>-0.73</td>
<td>1.504</td>
<td>-0.07</td>
<td>1.505</td>
</tr>
<tr>
<td>(y)</td>
<td>0.100</td>
<td>8.70</td>
<td>0.100</td>
<td>8.70</td>
<td>0.092</td>
</tr>
<tr>
<td>(Nu_{\text{min}})</td>
<td>0.700</td>
<td>1.16</td>
<td>0.694</td>
<td>0.29</td>
<td>0.692</td>
</tr>
<tr>
<td>(y)</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 3.1: Comparison of thermal and flow quantities with benchmark solutions of De Vahl Davis (1983) for \(P=0.71, Ra=10^3\).
<table>
<thead>
<tr>
<th>Property</th>
<th>20x20</th>
<th>% error</th>
<th>40x40</th>
<th>% error</th>
<th>60x60</th>
<th>% error</th>
<th>Bench mark</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{\text{max}}$</td>
<td>16.172</td>
<td>-0.04</td>
<td>16.232</td>
<td>0.33</td>
<td>16.300</td>
<td>0.75</td>
<td>16.178</td>
</tr>
<tr>
<td>$y$</td>
<td>0.800</td>
<td>-2.90</td>
<td>0.825</td>
<td>0.24</td>
<td>0.817</td>
<td>-0.72</td>
<td>0.823</td>
</tr>
<tr>
<td>$v_{\text{max}}$</td>
<td>19.543</td>
<td>-0.38</td>
<td>19.689</td>
<td>0.37</td>
<td>19.723</td>
<td>0.54</td>
<td>19.617</td>
</tr>
<tr>
<td>$x$</td>
<td>0.100</td>
<td>-15.9</td>
<td>0.125</td>
<td>5.04</td>
<td>0.117</td>
<td>-1.70</td>
<td>0.119</td>
</tr>
<tr>
<td>$Nu$</td>
<td>2.227</td>
<td>-0.71</td>
<td>2.241</td>
<td>-0.09</td>
<td>2.245</td>
<td>0.09</td>
<td>2.243</td>
</tr>
<tr>
<td>$Nu_{1/2}$</td>
<td>2.228</td>
<td>-0.67</td>
<td>2.241</td>
<td>-0.09</td>
<td>2.263</td>
<td>0.89</td>
<td>2.243</td>
</tr>
<tr>
<td>$Nu_0$</td>
<td>2.202</td>
<td>-1.61</td>
<td>2.234</td>
<td>-0.18</td>
<td>2.223</td>
<td>-0.67</td>
<td>2.238</td>
</tr>
<tr>
<td>$Nu_{\text{max}}$</td>
<td>3.430</td>
<td>-2.78</td>
<td>3.503</td>
<td>-0.71</td>
<td>3.490</td>
<td>-1.08</td>
<td>3.528</td>
</tr>
<tr>
<td>$y$</td>
<td>0.150</td>
<td>4.80</td>
<td>0.150</td>
<td>4.80</td>
<td>0.150</td>
<td>4.80</td>
<td>0.143</td>
</tr>
<tr>
<td>$Nu_{\text{min}}$</td>
<td>0.598</td>
<td>2.05</td>
<td>0.588</td>
<td>0.34</td>
<td>0.586</td>
<td>0.00</td>
<td>0.586</td>
</tr>
<tr>
<td>$y$</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 3.2: Comparison of thermal and flow quantities with benchmark solutions of De Vahl Davis (1983) for $P=0.71$, $Ra=10^4$.

<table>
<thead>
<tr>
<th>Property</th>
<th>20x20</th>
<th>% error</th>
<th>40x40</th>
<th>% error</th>
<th>60x60</th>
<th>% error</th>
<th>Bench mark</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{\text{max}}$</td>
<td>34.367</td>
<td>-1.05</td>
<td>34.461</td>
<td>-0.77</td>
<td>34.607</td>
<td>-0.35</td>
<td>34.730</td>
</tr>
<tr>
<td>$y$</td>
<td>0.850</td>
<td>-0.60</td>
<td>0.850</td>
<td>-0.60</td>
<td>0.850</td>
<td>-0.60</td>
<td>0.855</td>
</tr>
<tr>
<td>$v_{\text{max}}$</td>
<td>67.221</td>
<td>-2.00</td>
<td>68.464</td>
<td>-0.18</td>
<td>68.909</td>
<td>0.47</td>
<td>68.590</td>
</tr>
<tr>
<td>$x$</td>
<td>0.050</td>
<td>-24.2</td>
<td>0.075</td>
<td>13.63</td>
<td>0.067</td>
<td>1.5</td>
<td>0.066</td>
</tr>
<tr>
<td>$Nu$</td>
<td>4.415</td>
<td>-2.30</td>
<td>4.488</td>
<td>-0.69</td>
<td>4.508</td>
<td>-0.24</td>
<td>4.519</td>
</tr>
<tr>
<td>$Nu_{1/2}$</td>
<td>4.398</td>
<td>-2.68</td>
<td>4.481</td>
<td>-0.84</td>
<td>4.504</td>
<td>-0.33</td>
<td>4.519</td>
</tr>
<tr>
<td>$Nu_0$</td>
<td>4.506</td>
<td>-0.07</td>
<td>4.450</td>
<td>-1.31</td>
<td>4.486</td>
<td>-0.51</td>
<td>4.509</td>
</tr>
<tr>
<td>$Nu_{\text{max}}$</td>
<td>7.419</td>
<td>-3.86</td>
<td>7.400</td>
<td>-4.11</td>
<td>7.552</td>
<td>-2.14</td>
<td>7.717</td>
</tr>
<tr>
<td>$y$</td>
<td>0.100</td>
<td>23.5</td>
<td>0.075</td>
<td>-7.4</td>
<td>0.083</td>
<td>2.5</td>
<td>0.081</td>
</tr>
<tr>
<td>$Nu_{\text{min}}$</td>
<td>0.793</td>
<td>8.78</td>
<td>0.729</td>
<td>0.00</td>
<td>0.724</td>
<td>-0.69</td>
<td>0.729</td>
</tr>
<tr>
<td>$y$</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 3.3: Comparison of thermal and flow quantities with benchmark solutions of De Vahl Davis (1983) for $P=0.71$, $Ra=10^5$. 
Table 3.4: Comparison of thermal and flow quantities with benchmark solutions of De Vahl Davis (1983) for $P=0.71$, $Ra=10^6$.

\[
h(x,t) = \sum_{n=-N}^{N} a_n(t)e^{ikx},
\]

(3.55)

where $2N$ is the total number of grid points in the streamwise direction and $a_n$ is the spectral coefficient. We compare the growth of the first four harmonics and the results are shown in Fig. 3.3 for $G=1$, $S=100$, $P=7.02$, $M=35.1$, $Bi=1.0$ and $k=k_M$, where $k_M$ is the wavenumber for maximum linear growth (see Sect. 4.3). Other parameters are explained in Chapter 2. From the Fig. 3.3, we observe that all the first four harmonics stay in good agreement up to $t=1100$ which shows the accuracy of the code.
Figure 3.3: Evolution of first four harmonic modes is compared between full-scale computation and long-wave theory for $G=1$, $S=100$, $P=7.02$, $M=35.1$, $Bi=1$, and $k=0.0677$. The fundamental mode (top curve) and lowest harmonics stay in good agreement up to $t=1100$. 
Chapter 4

Rupture in Horizontal Layers

In this chapter, the rupture dynamic of a horizontal film on a heated substrate has been studied by integrating the fully-coupled nonlinear system of continuity, momentum, and energy equations. The system is solved using finite-element method in an Arbitrary Lagrangian Eulerian frame of reference to update precisely the motion of the interface. The results of these simulations are compared with those from the long-wave theory. Fully nonlinear process of spontaneous rupture due to thermocapillarity is shown for the first time.

4.1 Introduction

A liquid layer placed on a horizontal heated plate can become unstable due to various hydrodynamic instability mechanisms. When the layer is thin, the interfacial mode of thermocapillary instability is particularly important; the instability due to buoyancy and the Pearson mode of thermocapillary instability are absent (Williams & Davis, 1982; Goussis & Kelly, 1990). Unlike that of the Pearson type, the interfacial mode requires free-surface deformations. Since the surface tension suppresses disturbances with short wavelength, the interfacial mode occurs in the form of long surface waves. The dynamics of the flow then can be adequately described by the long-wave theory, (Benney, 1966) which assumes that the temporal and spatial variations of the flow are slow (lubrication approximation).

Many previous studies of nonlinear flow developments in thin heated films thus have been performed using the long-wave theory (Burelbach, Bankoff & Davis, 1988;
Joo, et al., 1991, Joo, Davis & Bankoff, 1993). In this method, the governing system of coupled equations is collapsed into a single evolution equation (Eq. 2.85) for the local film thickness. The evolution of the layer can be studied by integrating this equation. However, near rupture, the inertial effects become significant and thus the evolution equation becomes inappropriate.

If one wishes to study the rupture dynamics properly, one must instead integrate the complete system of continuity, momentum and energy equations with full nonlinear free-surface conditions. To this end, we introduce an unsteady Finite Element Method (FEM) with Chorin-type Fractional Step Method for temporal discretization and the Arbitrary Lagrangian Eulerian (ALE) description for accurate update of the moving boundary. The numerical scheme used is discussed in detail in Chapter 3. In this chapter, we confirm the fingering process reported via long-wave theory, and further examine, for the first time, the fully-nonlinear process of spontaneous film rupture.

First, the governing equations and the boundary conditions are explained for a two-dimensional flow in Sect. 4.2 and the method of analysis in Sect. 4.3. The results from the spectral computation of evolution equation are discussed in Sect. 4.4 and the use of full-scale computation is justified. In Sect. 4.5, we will illustrate the fingering process via full-scale computation. The influences of the Biot number, the Marangoni number and the Prandtl number are discussed in Sect. 4.6. Finally, in Sect. 4.7, we examine Pearson mode instability in a thick liquid layer and conclude in Sect. 4.8.

4.2 Governing Equations

In Chapter 2, the governing equations are shown for a three-dimensional flow. In this and the next chapter, dynamics of a thin film in a two-dimensional domain
is discussed. Therefore, we will rewrite the governing equations. This is achieved by considering an infinitely long domain in the spanwise \((y)\) direction so that the gradients in this coordinate direction vanish, \(i.e., \partial / \partial y = 0\). The governing equations are:

**Conservation of mass:**

\[
\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0, \tag{4.1}
\]

**Conservation of momentum:**

\[
\frac{\partial u}{\partial t} + (u - g_z \frac{\partial u}{\partial x}) + (w - g_z \frac{\partial u}{\partial z}) = -\frac{\partial p}{\partial x} + G\sin \beta + \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2} \right), \tag{4.2}
\]

\[
\frac{\partial w}{\partial t} + (u - g_z \frac{\partial w}{\partial x}) + (w - g_z \frac{\partial w}{\partial z}) = -\frac{\partial p}{\partial z} - G\cos \beta + \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} \right), \tag{4.3}
\]

**Conservation of energy:**

\[
\frac{\partial \theta}{\partial t} + (u - g_z \frac{\partial \theta}{\partial x}) + (w - g_z \frac{\partial \theta}{\partial z}) = \frac{1}{P} \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial z^2} \right). \tag{4.4}
\]

Here, \(G\) is the Galileo number and \(P\) is the Prandtl number. We use a Cartesian coordinate system \((x,z)\), with \(x\)-axis directed downstream and the \(z\)-axis into the liquid from the bottom plate. The origin of the system is assumed located at the corner of the plate. Note that the above equations are written in an ALE frame of reference.

At the liquid-air interface, \(z = h(x,t)\), we need to satisfy the kinematic, tangential- and normal-stress conditions, and the energy balance. The height of the interface changes in streamwise location and time, and is defined by the kinematic equation:

\[
\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} = w. \tag{4.5}
\]

The normal component of the surface traction is balanced by the capillary force:
\[-p + \frac{2}{N^2} \left[ \left( \frac{\partial h^2}{\partial x} - 1 \right) \frac{\partial u}{\partial x} - \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] = \frac{3S}{N^3} \left( 1 + \frac{\partial^2 h^2}{\partial x^2} \right), \tag{4.6}\]

where,

\[N = \left( 1 + \frac{\partial h^2}{\partial x} \right)^{\frac{1}{2}}, \tag{4.7}\]

and \(S\) is the surface tension number. The shear stress at the interface is affected by the thermocapillarity, and can be expressed as:

\[\left( 1 - \frac{\partial h^2}{\partial x} \right) \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) - \frac{4}{\partial x} \frac{\partial u}{\partial x} \frac{\partial h}{\partial x} = \frac{2NM}{P} \left( \frac{\partial \theta}{\partial x} + \frac{\partial h \partial \theta}{\partial x \partial z} \right), \tag{4.8}\]

where, \(M\) is the Marangoni number. The energy balance gives:

\[\frac{\partial h \partial \theta}{\partial x \partial x} - \frac{\partial \theta}{\partial z} + \frac{\partial \theta}{\partial x} = 0, \tag{4.9}\]

where, \(Bi\) is the Biot number.

The computations are done in one spatial period

\[L = \frac{2\pi}{k}, \tag{4.10}\]

where \(k\) is the wavenumber of the imposed disturbance. No-slip and constant temperature boundary conditions are applied on the plate:

\[\begin{align*}
  &u(x, 0, t) = 0, \\
  &w(x, 0, t) = 0,
\end{align*} \tag{4.11}\]

\[\theta(x, 0, t) = 1. \tag{4.12}\]

A periodic boundary condition is applied for the variables \(u, w, p\) and \(\theta\).

\[\begin{align*}
  &u(0, y, t) = u(L, y, t), \\
  &w(0, y, t) = w(L, y, t), \\
  &p(0, y, t) = p(L, y, t), \\
  &\theta(0, y, t) = \theta(L, y, t).
\end{align*} \tag{4.13}\]
4.3 Method of Analysis

We perturb the free surface at time \( t=0 \) and study the nonlinear evolution of the disturbance in time. The perturbation wavenumber is selected using the linear theory. For this purpose, we have to solve the Orr-Sommerfeld equation numerically. However, an analytical expression for the cut-off wavenumber can be obtained by performing a linear analysis on the long-wave evolution equation. This is valid only for small Reynolds number flow (\( G \sim O(1) \)). Since the present study is focused on the flow of extremely thin layers, we follow this approach. In this approach, a simple harmonic disturbance of small amplitude is substituted in the evolution equation (Eq. 2.85) and is linearized. The following expressions result (Joo, et.al., 1991):

\[
\Gamma = k^2 \left[ \frac{BiM}{P} \left( \frac{d}{1 + dB} \right)^2 + \frac{2G^2}{15} d^6 \sin^2 \beta - \frac{G}{3} \cos \beta - k^2 Sa \right], \quad (4.14)
\]
is the effective growth rate and

\[
c = Ga^2 \sin \beta, \quad (4.15)
\]
is the linearized phase speed. The growth rate is influenced by the destabilizing effect of thermocapillary and inertia, and the stabilizing effects of hydrostatic pressure and surface tension. The cut-off wavenumber is obtained by setting \( \Gamma = 0 \).

\[
k_c = \left\{ \frac{1}{Sa^3} \left[ \frac{BiM}{P} \left( \frac{d}{1 + dB} \right)^2 + \frac{2G^2}{15} d^6 \sin^2 \beta - \frac{G}{3} \cos \beta \right] \right\}^{\frac{1}{2}}, \quad (4.16)
\]
The maximum growth rate occurs at \( k = k_M = k_c / \sqrt{2} \). The condition for instability is \( \Gamma > 0 \).

In full-scale computation, the stability of the system is analyzed by perturbing the free surface with a sinusoidal disturbance,

\[
h(x, 0) = 1 + 0.1 \cos(kx), \quad (4.17)
\]
where $k$ is the wavenumber selected from Eq. 4.16. The integration is done on one spatial period. In this way, the superharmonics, disturbances of wavelength $\lambda$, $\lambda/2$, $\lambda/4 \cdots$, are allowed to grow and interact nonlinearly. This is also known as study of superharmonic instability. The results are presented with the film thickness $h(x,t)$ and its spatial spectral coefficient $a_n(t)$ defined as

$$h(x,t) = \sum_{n=-N}^{n=N} a_n(t)e^{i n k x}, \quad (4.18)$$

where $2N$ is the number of grid points in the streamwise direction. Integration is terminated when the local minimum becomes less than 1% of initial mean thickness, at which moment rupture is assumed. We assume that beyond this point molecular forces become important and our governing system will be insufficient for the accurate description of ensuing physics. However, the molecular force of attraction will eventually break the film (Burrelch, et.al., 1988). When the film does not rupture, we continue the integration, while monitoring the Fourier modes of the surface wave, until a saturated state is reached. If the magnitude of each mode, $|a_n|$, ceases to fluctuate, we assume that the interface has obtained a saturated wave form traveling downstream. If the modes continue to oscillate in a quasi-periodic or an aperiodic manner, a quasi-periodic or a chaotic state is assumed.

The computational domain is discretized into non-overlapping three-node linear-triangular elements. One such mesh, at the point of rupture, is shown in Fig. 4.1. The solution depends highly on the mesh resolution. Therefore, a grid-convergence study is conducted for different cases simulated to ensure complete capturing of even small-scale structures that develop when the film ruptures. In Fig. 4.2 results from one such study is shown for $G=1$, $S=100$, $P=7.02$, $M=35.1$, $Bi=1.0$, $\beta=0$ and $k=k_M$. In these figures, the instantaneous free-surface configuration is shown at different time levels. These figures clearly prove that the spectral computation of kinematic equation preserves the symmetry of the free surface even with a coarse grid.
Figure 4.1: Typical finite element mesh at the time of rupture ($t_R$) is shown in (a), (b), and (c) when $k=k_M$, $k_M/2$, and $k_M/4$, respectively. The parameters used in the simulation are $G=1$, $S=100$, $P=7.02$, $M=106.2$, $Bi=0.1$, $k_M=0.0677$, and $\beta=0^\circ$. 
Figure 4.2: \( G=1, \ S=100, \ P=7.02, \ M=35.1, \ Bi=1, \) and \( k_M=0.0677. \) Snapshot of the free surface at the intervals of 100 viscous time units is shown (a) when the computation domain of 33 grid points in the streamwise direction and 11 grid points in the z-direction is used, and similarly in (b) for a 65x11 mesh, and in (c) for a 129x11 mesh. This study shows that the 65x11 grid is sufficient for this particular problem. The minimum \( (h_{\text{min}}) \) and the maximum \( (h_{\text{max}}) \) local film thickness at the time of rupture \( (t_{\text{final}}) \) are also shown.

(.....) Free-surface shape at \( t=0, \ (-.-.-.) \) Free-surface shape at \( t=t_{\text{final}} \)
A grid size of 65 grid points in the $x$-direction and 11 grid points in the $y$-direction is sufficient for this particular study. Subsequently, twice or four times this mesh size is used, respectively, when the wavenumber is $k_M/2$ or $k_M/4$. Increasing the spatial resolution further does not alter the figures shown.

### 4.4 Fingering Process via Long-Wave Evolution Equation

For a horizontal layer, $\beta=0$, long wave evolution equations can be expressed as:

$$
\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left[ \left\{ \frac{BiM}{P} \left( \frac{h}{1 + Bi h} \right)^2 - \frac{G}{3} h^3 \right\} \frac{\partial h}{\partial x} + Sh^3 \frac{\partial^3 h}{\partial x^3} \right] = 0,
$$

(4.19)

where $h(x,t)$ is the film thickness at horizontal location $x$ (in units of the mean film thickness $d$) and time $t$ (in units of $d^2/\nu$, where $\nu$ is the kinematic viscosity). The parameters, the layer thickness $G$, the heat-transfer coefficient across the free surface $Bi$, thermocapillarity $M$, Prandtl number $P$, and mean surface tension $S$ are defined in Chapter 2. The second term in Eq. 4.19 describes thermocapillary effects, and is destabilizing when the layer is heated from below ($M>0$). The last two terms, respectively, represent the stabilizing effects of hydrostatic pressure and mean surface tension.

Numerical integration of Eq. 4.19 shows growth of long enough disturbances ($k<k_c$, where $k$ and $k_c$ are disturbance wavenumber and cutoff wavenumber due to capillarity) for large enough temperature gradient ($BiM/P(1 + Bi)^2 > G/3$), in agreement with linear stability analysis. As the disturbance amplitude grows further, higher harmonics are generated and grow rapidly. Contrary to draining films, where the disturbance waves propagate downstream, in a horizontal layer, there is no nonlinear saturation into periodic or steady states. Disturbances appear to grow until the film ruptures. Figure 4.3 shows the surface evolution for three different wavenumbers, $k_M$ that corresponds to the maximum linear growth rate, $k_M/2$, and
Figure 4.3 (a) $k=k_M$
Final state: Likely to Rupture
\[ t_{\text{final}} = 1160.0 \]
\[ h_{\text{min}} = 0.0661 \]
\[ h_{\text{max}} = 2.4160 \]

Figure 4.3 (b) $k=k_M/2$
Final state: Likely to Rupture
\[ t_{\text{final}} = 2265.0 \]
\[ h_{\text{min}} = 0.1412 \]
\[ h_{\text{max}} = 2.2968 \]
Figure 4.3 (c) \( k = k_M / 4 \)
Final state: Likely to Rupture

\[
\begin{align*}
    t_{\text{final}} &= 4400.0 \\
    h_{\text{min}} &= 0.1273 \\
    h_{\text{max}} &= 1.7777
\end{align*}
\]

Figure 4.3: \( G=1, S=100, P=7.02, M=35.1, Bi=1, \) and \( k_M = 0.0677 \). In figures (a), (b) and (c), the instantaneous free-surface configuration at the intervals of 50, 100, and 200 viscous time units and the corresponding growth in the harmonic modes are shown, when the disturbance wavenumbers are \( k_M, k_M / 2 \) and \( k_M / 4 \), respectively. These results are obtained from the spectral computation of fully-nonlinear long-wave evolution equation. The minimum \( h_{\text{min}} \) and the maximum \( h_{\text{min}} \) local film thickness at the time \( t = t_{\text{final}} \) are also shown.

(......) Free-surface shape at \( t = 0 \), (-.-.-.) Free-surface shape at \( t = t_{\text{final}} \),
Modes representation: (—) \( n = 1 \); (-.-.-.) \( n = 2 \); (- - -) \( n = 3 \); (.....) \( n = 4 \)

\( k_M / 4 \). Each line represents a snapshot of the surface shape, and the computation is terminated when the shape cannot be resolved with sufficiently large (up to 64) independent Fourier modes, an indication of violation of the long-wave theory. The numerical scheme used is a pseudo-spectral method with semi-implicit time-marching, discussed in detail by Joo, et.al. (1991). In all the three cases shown,
there is a secondary flow development in the form of fingers, which is due to the
growth of higher harmonics. Figure 4.3 shows that the fingering occurs in an earlier
stage, if the disturbance wave is longer. It also indicates the possibility of multiple
rupture spots per initial period. In the incipient rupture process, however, the local
free-surface slope increases continuously, eventually violating the basic assumption
required by Eq. 4.19. The inertial effects, assumed to be small in Eq. 4.19, also
becomes significant. The evolution equation thus becomes inappropriate before the
rupture occurs.

4.5 Fingering Process via Full-Scale Computation

Consider a layer of constant property liquid kept on a horizontal plate maintained
at a constant temperature $T_w$. The film is unbounded horizontally, but bounded
above by its interface with the air of far-field temperature $T_i(< T_w)$. The heat
conducted across the liquid layer is lost through the interface due to convection.
We assume that surface tension decreases linearly with temperature. The governing
equations are two-dimensional conservation laws for mass, momentum and energy.
The control parameters of the problem are the Galileo number ($G$), Marangoni
number ($M$), Prandtl number ($P$) and the Biot number ($Bi$). No-slip boundary
condition is applied at the bottom and periodic boundary conditions are imposed
in the horizontal direction. On the liquid-air interface, continuity of normal and
tangential stresses and energy balance are applied. From Eq. 4.19, we note that the
thermocapillarity is characterized by $(Bi M/P (1 + Bi)^2)$. We fix a value of 1.25 to
this parameter, and set $G=1$ and $S=100$.

Figure 4.4 shows the surface evolution and the growth of its harmonic modes
for three different wavenumbers $k_M$, $k_M/2$, and $k_M/4$ with $Bi=1$. Initially, the film
grows exponentially according to the linear theory. Energy is confined to the
Figure 4.4 (a) $k=k_M$
Final state: Rupture
$t_R=1268.6$
$h_{\text{min}}=0.0099$
$h_{\text{max}}=2.3922$

Figure 4.4 (b) $k=k_M/2$
Final state: Rupture
$t_R=2491.3$
$h_{\text{min}}=0.0099$
$h_{\text{max}}=2.4469$
Figure 4.4 (c) \( k = k_M/4 \)

Final state: Rupture

\[
\begin{align*}
    t_R &= 4974.1 \\
    h_{\text{min}} &= 0.0099 \\
    h_{\text{max}} &= 2.4049 
\end{align*}
\]

Figure 4.4: \( G=1, \ S=100, \ P=7.02, \ M=35.1, \ Bi=1, \) and \( k_M=0.0677 \). In figures (a), (b) and (c), the instantaneous free-surface configuration at the intervals of 50, 100, and 200 viscous time units and the corresponding growth in the harmonic modes are shown, when the disturbance wavenumbers are \( k_M, \ k_M/2 \) and \( k_M/4 \), respectively. These results are obtained from direct-numerical (FEM) simulation. The minimum (\( h_{\text{min}} \)) and the maximum (\( h_{\text{max}} \)) local film thickness at the time of rupture (\( t_R \)) are also shown.

(......) Free-surface shape at \( t=0 \), (.-.-,-) Free-surface shape at \( t=t_R \)

Modes representation: (—) \( n=1 \); (.-.-,-) \( n=2 \); ( - - - ) \( n=3 \); (......) \( n=4 \)

fundamental mode and the interface maintains its simple-harmonic shape. As time progresses, thermocapillarity becomes significant. This drives the fluid from the hotter troughs to the relatively colder crests and thereby causing the liquid layer to become thinner and thinner at the trough. Now the energy is no longer confined to the fundamental mode but has spread to its superharmonics. As the interface
approaches the solid wall, viscous effects become dominant and the thin layer flattens due to the resistance offered by the solid wall. The two edges of the flattened region have large slope and positive curvature and are drawn downward by the capillary pressure. These edges grow as fingers or new troughs. Meanwhile, the thermocapillary convection induces high velocities toward the wall and the fluid starts draining outwards. However, the fluid near the central region is trapped between two new troughs, that are at high pressure, is pushed upwards to conserve mass and grows as a new crest. The downward growing fingers ultimately touch the plate and break the film. If the flow were isothermal, initial disturbance would have been suppressed after initial transients. This implies that with sufficient heating, the thermocapillarity overcomes the hydrostatic and capillary stabilizations and breaks the film.

As is seen, dynamical thinning leading to spontaneous rupture occurs in the form of "fingers," and at that moment energy is no longer confined to the fundamental mode but has spread to its harmonics. There is no nonlinear saturation into periodic or steady state. For longer waves, Figs. 4.4(b) and (c), there are multiple rupture spots. This clearly confirms that the "fingering" process leading to breaking of the thin film is not an artifact of long-wave theory but an actual physical phenomenon. Indeed, by integrating full system of equations, we are able to accurately follow the dynamics until the film ruptures.

A quantitative comparison between the long-wave approximation and the full system is made in Fig. 4.5, where the first four Fourier modes are plotted for the evolutions shown in Figs. 4.3 and 4.4. For clarity, a logarithmic scale is used. During the initial stage of the evolution, the local free-surface slope is small everywhere, and the long-wave approximation agrees well with the computation of the full system. The fundamental mode (top curve) and lowest harmonics stay in good agreement
Figure 4.5: Evolution of first four harmonic modes is compared between full-scale computation and long-wave theory when $G=1$, $S=100$, $P=7.02$, $M=35.1$, $Bi=1$, and $k_M=0.0677$ for $k=k_M$ in (a), $k=k_M/2$ in (b) and for $k=k_M/4$ in (c). The fundamental mode (top curve) and lowest harmonics (bottom curve) stay in good agreement up to $t=1100$ for $k=k_M$, $t=2100$ for $k_M/2$, and $t=3500$ for $k_M/4$. This also illustrates that the long-wave theory based on lubrication type approximation agrees very well with the full-scale computation over a long period of evolution except near rupture.

(---) Finite-Element Method; (....) Long-Wave Evolution Equation
up to \( t=1100 \) for \( k=k_M \), up to \( t=2100 \) for \( k=k_M/2 \), and up to \( t=3500 \) for \( k=k_M/4 \). The higher harmonics start to diverge significantly sooner. Except near rupture, the long-wave theory shows surprisingly good qualitative agreement.

4.6 Influence of Biot Number and \( M/P \)

Thermocapillarity is absent if \( Bi=0 \) or \( \infty \) and in effect, the interface obtains the temperature of the bottom plate \( T_w \) or the ambient temperature \( T_s \) respectively. As can be seen from Eq. 4.14, at \( Bi=1 \) thermocapillarity reaches a maximum. Consequently, if we reduce the Biot number to 0.1 in our previous simulations, we reduce the thermocapillarity and retard rupture. This is evident from Fig. 4.6, where the free-surface evolution through full-scale computation is plotted. Here, we retain the value of \( (BiM/P(1 + Bi)^2) \) as 1.25, reduce the \( Bi \) to 0.1 and change \( M/P \) accordingly. As noted before, initially the perturbation grows exponentially, consistent with the linear theory, and the free surface maintains the simple harmonic shape. Soon, dimples appear at the surface. Their locations have moved further away from the trough of the initial perturbation, and breaking occurs at multiple spots.

The tangential stress condition suggests that in these flows, the ratio \( M/P \) is an important parameter in studying the dynamics of the flow. So in Fig. 4.7, the evolution of the free surface for three different wavenumbers, \( k_M, k_M/2, \) and \( k_M/4 \), are shown for \( P=0.01 \) with \( M/P=5 \) and \( (BiM/P(1 + Bi)^2) = 1.25 \). We notice there is no change in the dynamics including the rupture time. The rupture time, for all the cases discussed above, is recorded and listed in Table (4.1).
Finite Element Method
Final state: Rupture
\[ t_{\text{final}} = 2414.6 \]
\[ h_{\text{min}} = 0.0099 \]
\[ h_{\text{max}} = 2.4076 \]

Long-wave theory
Final state: Likely to rupture
\[ t_{\text{final}} = 1700.0 \]
\[ h_{\text{min}} = 0.1259 \]
\[ h_{\text{max}} = 2.2285 \]

Figure 4.6 (a) \( k = k_M \)
Finite Element Method
Final state: Rupture
\( t_{final} = 3386.9 \)
\( h_{min} = 0.0099 \)
\( h_{max} = 2.8326 \)

Long-wave theory
Final state: Likely to rupture
\( t_{final} = 2255.0 \)
\( h_{min} = 0.2752 \)
\( h_{max} = 2.3659 \)

Figure 4.6 (b) \( k = k_M / 2 \)
Figure 4.6 (c) $k=k_M/4$

Figure 4.6: $G=1$, $S=100$, $P=7.02$, $M=106.2$, $Bi=0.1$, and $k_M=0.0677$. In figures (a), (b) and (c), the instantaneous free-surface configuration at the intervals of 100, 100, and 200 viscous time units and the corresponding growth in the harmonic modes are shown, when the disturbance wavenumbers are $k_M$, $k_M/2$ and $k_M/4$, respectively. Results from both full-scale computation (FEM) and spectral computation of long-wave evolution equation are shown. The minimum ($h_{min}$) and the maximum ($h_{max}$) local film thickness at the time $t=t_{final}$ are also shown.

(-----) Free-surface shape at $t=0$, (-.-.-.) Free-surface shape at $t=t_{final}$

Modes representation: (-) $n=1$; (-.-.) $n=2$; (- - -) $n=3$; (.....) $n=4$
Figure 4.7 (a) $k=k_M$
Final state: Rupture

$t_{final}=1260.7$
$h_{min}=0.0099$
$h_{max}=2.3856$

Figure 4.7 (b) $k=k_M/2$
Final state: Rupture

$t_{final}=2483.3$
$h_{min}=0.0099$
$h_{max}=2.4331$
Figure 4.7 (c) \( k=k_M/4 \)

Final state: Rupture

\[ t_{\text{final}}=4956.3 \quad h_{\text{min}}=0.0099 \quad h_{\text{max}}=2.3973 \]

Figure 4.7: \( G=1 \), \( S=100 \), \( P=0.01 \), \( M=0.05 \), \( Bi=1.0 \), and \( k_M=0.0677 \). In figures (a), (b) and (c), the instantaneous free-surface configuration at the intervals of 50, 100, and 200 viscous time units and the corresponding growth in the harmonic modes are shown, when the disturbance wavenumbers are \( k_M \), \( k_M/2 \) and \( k_M/4 \), respectively. These results are obtained from direct-numerical (FEM) simulation. The minimum \( (h_{\text{min}}) \) and the maximum \( (h_{\text{min}}) \) local film thickness at the time of rupture \( (t_R) \) are also shown.

(-----) Free-surface shape at \( t=0 \), (-.-.-.) Free-surface shape at \( t=t_R \)

Modes representation: (---) \( n=1 \); (-.-.-.) \( n=2 \); (- - -) \( n=3 \); (-----) \( n=4 \)

<table>
<thead>
<tr>
<th>( k )</th>
<th>( B=1, P=7.02, M=35.1 )</th>
<th>( B=1, P=0.01, M=0.05 )</th>
<th>( B=0.1, P=7.02, M=106.18 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_m )</td>
<td>1268.62</td>
<td>1260.70</td>
<td>2414.63</td>
</tr>
<tr>
<td>( k_m/2 )</td>
<td>2491.29</td>
<td>2483.34</td>
<td>3386.93</td>
</tr>
<tr>
<td>( k_m/4 )</td>
<td>4974.88</td>
<td>4956.33</td>
<td>5462.35</td>
</tr>
</tbody>
</table>

Table 4.1: The rupture time in viscous time units is listed for \( eG=1 \), \( S=100 \), and \( (BiM/P)[d/(Bi + d)]^2=1.25 \). This is calculated using the criterion that local film thickness becomes 1% of initial mean thickness \( d \).
4.7 Thick Horizontal Layers: Pearson Mode Instability

In a heated layer, as the thickness of the film increases, the flow becomes stable due to hydrostatic stabilization. With further increase in the thickness, the flow becomes unstable again due to Pearson mode of thermocapillary instability. This stability window was identified by Kelly, Goussis & Davis (1986). Similarly, the Pearson mode appears at very high intensity of heating also. As reported by Goussis & Kelly (1990, 1991), this mode occurs if

\[
\frac{M}{Bi} > 16.04. \tag{4.20}
\]

In these flows, the interaction between the basic temperature field and the perturbation velocity field cause the instability. The convection is dominant and supplies energy for the disturbances to grow.

Pearson mode of instability in a thick layer is illustrated in Fig. 4.8 for \( G=100, S=465, Bi=1, P=7.02, M=600 \) and \( \beta=0 \). Here, as time progresses, the free-surface deformation disappears and the interface stays relatively flat. However, thermocapillarity is still dominant and longitudinal convective rolls appear near the interface. We do not observe rupture in this case.

Pearson mode of instability at very high intensity of heating is shown in Fig. 4.9. In this case, the thickness is held constant by fixing \( G \) and the intensity of heating is varied by changing \( M \). When heating is small, the interfacial mode of thermocapillarity is dominant, and the film ruptures via fingering mechanism. As the heating is increased, interfacial mode affects the growth only during the initial period. After initial transients, the thermal convection inside the liquid layer becomes dominant and so becomes the Pearson mode of instability. Subsequently, this induces large temperature gradient along the interface, and enhances the
Figure 4.8 (a) Free-surface shape
\[ t_{\text{final}} = 0.02 \quad h_{\text{min}} = 0.9999 \quad h_{\text{max}} = 1.0001 \]

Figure 4.8 (b) Velocity Vector at \( t = t_{\text{final}} \)

Figure 4.8 (c) Isothermal Contour at \( t = t_{\text{final}} \)

Figure 4.8: \( G = 100 \), \( S = 465 \), \( P = 7 \), \( M = 600 \), \( Bi = 1 \), and \( k = 6.28 \). This is a case of a thick film. A disturbance, whose wavelength equal to the thickness of the film is imposed initially. In (a), the instantaneous free-surface configuration at the intervals of 0.005 viscous time units, in (b) the final state with longitudinal rolls near the interface, and in (c) the isothermal lines at \( t = t_{\text{final}} \) are shown.

(.....) Free-surface shape at \( t = 0 \), (-.-.-.) Free-surface shape at \( t = t_R \)
Figure 4.9 (a) $\frac{BiM}{P} = 50$

Final state: Rupture $t_{final} = 6.5133$ $h_{min} = 0.0099$ $h_{max} = 2.0437$

Figure 4.9 (b) $\frac{BiM}{P} = 200$

Final state: Continuous Film $t_{final} = 11.9325$ $h_{min} = 0.6614$ $h_{max} = 1.3579$

Figure 4.9: $G=1$, $S=100$, $P=7$, $Bi=0.1$, $k=k_M$, and $\beta=0^\circ$. The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown in (a) and (b), respectively, for $\frac{BiM}{P} = 50$ and 200. In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented. Modes representation: (—) $n=1$; (---) $n=2$; ( - - - ) $n=3$; (.....) $n=4$
thermocapillarity. However, the surface flow is not able to penetrate the base flow and no severe local thinning occurs. This indicates that there exists of a window of heating intensity for rupture.

4.8 Conclusion

We conclude, that numerical simulation of dynamical thinning and spontaneous rupture of horizontal heated films agree qualitatively with the long-wave theory. The wavenumber $k=k_m$ leads to minimal rupture time. On the other hand, reducing Biot number from its critical value retards rupture. This phenomenon is particularly significant when $k=k_M$. Detailed rupture dynamics, including the rupture time, is described more accurately than in previous reports, since the governing equations are solved in a fully-coupled manner without any assumption.

In thin-layers, rupture occurs for a sufficient amount of heating. As the intensity of heating is increased, the Pearson mode becomes dominant due to increased convection inside the layer. This enhances the thermocapillarity by inducing large temperature gradient along the interface. However, rupture does not occur. This shows that there exists a window of heating intensity for rupture. When the thickness increases, free-surface deformation weakens and the Pearson mode becomes dominant. In this case also, the film stays continuous. In the next chapter, the dynamics of an inclined layer under the combined influence of thermocapillary and surface-wave instabilities is discussed.
Chapter 5

Thermocapillary and Surface-wave Instability in Inclined Layers

A thin heated film draining on an inclined plane can either form waves and stay continuous, or go through a spontaneous rupture process forming rivulets. It is of great engineering importance to distinguish these two phenomena. Since rupture is a highly nonlinear, it can not be analyzed completely using weakly nonlinear theories. In this regard, we investigate the fully nonlinear dynamics of the flow by integrating the coupled system of conservation equations for mass, momentum and energy using a finite-element method. Through extensive numerical simulations, a series of phase diagrams depicting the boundaries between wavy but continuous film and ruptured film are presented, and the interplay among instability mechanisms involved is examined (Krishnamoorthy, Ramaswamy & Joo, 1996b).

5.1 Introduction

A liquid layer is susceptible to the thermocapillary instability when it is heated from below. There are two modes of thermocapillary instability. The first mode is associated with the interaction between the basic temperature field and the velocity perturbation, and manifest itself in the form of convective rolls as first identified by Pearson (1958). As reported by Goussis & Kelly (1991), this mode occurs either in relatively thick layers or at high intensity of heating, and the free-surface deformation is not required. The other mode is associated with the variation of the basic temperature with the surface deformation. This mode occurs in very thin layers and
causes severe surface deformation, often resulting in dry spots via rupture process. It was shown by Krishnamoorthy, et al. (1995) that a horizontal layer subjected to this interfacial mode of instability always ruptures.

When the liquid layer is tilted, it drains downstream and can become unstable even in the absence of heat transfer. This isothermal mode of instability is often called surface-wave instability and was first identified by Yih (1955,1963) and Benjamin (1957), who, through linear-stability analysis, reported the critical values for the inclination angle and the layer thickness. After the onset of the instability, surface waves exhibit a rich variety of nonlinear dynamics, which has been the subject of numerous recent studies. A comprehensive discussion of these works can be found in the review by Lin and Wang (1985) or more recently by Chang (1994). As long as the flow stays laminar, all surface waves appear to saturate to a periodic, a quasiperiodic, or a chaotic state. Evolution toward rupture has not been observed in isothermal film flows.

When the layer is tilted and heated, the interfacial mode of thermocapillary and the surface-wave instabilities coexist and dictate the dynamics of the flow in a competitive manner. When the thermocapillary (surface-wave) instability is dominant, the layer will rupture (saturate). It is of great practical importance to find the parameter ranges where these two distinctive phenomena (rupture and saturation) occur. For example, in film-cooling operation the waviness of the surface may be desirable for heat-transfer enhancement, but the rupture can be disastrous. It is the purpose of this study to distinguish these two phenomena for a heated draining film and give further insight to the underlying mechanism.

In this chapter, we systematically analyze the influence of the control parameters viz. film thickness, amount of heating, wavenumber of the imposed disturbance, angle of inclination and heat loss at the interface on the nonlinear dynamics of rup-
turing mechanism. Through an extensive parametric search, we identify the regions where the flow has the tendency to either saturate or rupture, and present a series of phase diagrams that depict the phase boundaries between these two flow behaviors. Systematic comparison with the isothermal flow is also furnished.

### 5.2 Method of Analysis

The method of analysis for an inclined layer is similar to what has been followed for a horizontal layer. We integrate the governing equations Eqs. 4.1 to 4.4 by posing an initial-value problem. A simple-harmonic disturbance of the form

\begin{equation}
    h(x, 0) = 1 + 0.1 \cos(kx),
\end{equation}

is imposed on the free surface and its evolution is studied in time. Here, \( k \) is the wavenumber of the perturbation and is selected based on the linear theory. The integration is done on one spatial period. The results are presented with the film thickness \( h(x,t) \) and its spatial spectral coefficient \( a_n(t) \) defined in Eq. 4.18. Integration is stopped at any moment when the minimum film thickness becomes less than 1\% of initial mean thickness, at which moment rupture is assumed. We assume that beyond this point molecular forces become important and our governing system will be insufficient for the accurate description of ensuing physics. When the film does not rupture, we continue the integration, while monitoring the Fourier modes of the surface wave, until a saturated state is reached. If the magnitude of each mode, \( |a_n| \), ceases to fluctuate, we assume that the interface has obtained a saturated wave-form traveling downstream. In this case, the interface obtains a stationary wave-form and the number of peaks will be determined by the dominant overtone. If the modes continue to oscillate in an aperiodic manner, a chaotic state is assumed.
The governing equations (Eqs. 4.1 to 4.4) and the boundary conditions (Eqs. 4.6, 4.8, and 4.9) suggest that the dynamics of the flow is determined by the following five parameters:

1. angle of inclination of the plate
2. initial mean thickness of the film
3. intensity of heating
4. heat loss at the interface and
5. wavenumber of the imposed disturbance.

In our calculation, these parameters can be changed by varying $\beta$, $G$, $M$, $Bi$, and $k$, respectively. In the following sections we will analyze systematically their influence on rupture mechanism. The numerical problem is highly dependent on the spatial and temporal resolution of computational domain. The results presented in the following sections are obtained after intensive grid-independence studies.

5.3 Combined Thermocapillary and Surface-Wave Instabilities

In an isothermal layer, the basic flat film solution (Eqs. 2.38 to 2.40) is unstable to a long waves. The linear stability analysis (Yih, 1955, 1963; Benjamin, 1957) defines a critical Reynolds number $G_c$ as:

$$G_c = \frac{5 \cot \beta}{2 \sin \beta},$$  

(5.2)

where $\beta$ is the angle of inclination. The above relation explains that the flow is always stable in a horizontal layer and is always unstable in a vertical layer. For a given film thickness, there is a cut-off angle below which the layer is always stable to
due the hydrostatic stabilization. However in nonisothermal flows, no cut-off angle exists and layer can becomes unstable at any angle of inclination due to the presence of thermocapillarity. In the following sequence, it is shown that as the inclination angle is increased, the evolution toward rupture is gradually replaced by that toward saturated wave.

Figure 5.1(a) shows the evolution of a horizontal film when \( \theta=1, \ S=100, \ Bi=0.1, \ M=350, \ P=7 \) and \( k = k_M \). Each line represents instantaneous free-surface configuration at the time shown. Results from both full-scale computation and spectral computation of long-wave evolution equation are shown for comparison. In this case, there is no mean flow, and only the thermocapillarity causes the instability. As discussed in the previous chapter, the film always ruptures after characteristic fingering associated with the lubrication pressure. In this case the thermocapillarity overcomes the hydrostatic stabilization, and induces rupture at two points. Figure 5.1(b) shows the evolution of the interface and the corresponding growth in the harmonic modes when \( \beta=10^\circ \). Corresponding isothermal

![Graphs showing the evolution of a horizontal film](image.png)

**Figure 5.1 (a) \( \beta=10^\circ \ k_M=0.1378 \)**

Final state: Rupture

- \( t_{final}=183.8 \)
- \( h_{min}=0.0099 \)
Figure 5.1 (b) $\beta=10$  $k_M=0.1380$

Final state: Rupture

$t_{final}=398.3$

$h_{min}=0.0099$

$h_{max}=2.2822$

Figure 5.1 (c) $\beta=30$  $k_M=0.1392$

Final state: Wavy, but Continuous

$t_{final}=502.5$

$h_{min}=0.1503$

$h_{max}=2.0055$
Figure 5.1 (d) β=60    $k_M=0.1426$
Final state: Wavy, but Continuous  $t_{final}=194.4$  $h_{min}=0.3038$  $h_{max}=1.7524$

Figure 5.1 (e) β=90    $k_M=0.1460$
Final state: Wavy, but Continuous  $t_{final}=196.9$  $h_{min}=0.3309$  $h_{max}=1.7258$

Figure 5.1: $G=1$, $S=100$, $P=7$, $M=350$, $Bi=0.1$, $k=k_M$. The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown for $β=0^\circ$, $10^\circ$, $30^\circ$, $60^\circ$, and $90^\circ$, respectively, in (a) to (e). In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented. Modes representation: (—) $n=1$; (---•--) $n=2$; ( - - - ) $n=3$; (.....) $n=4$
thin film is stable. Here due to the mean flow in the streamwise direction, the crest moves faster than the trough, steeping the slope behind the trough. Therefore, when the trough flattens and the edges bulge outward, the rear edge gains a larger curvature. It then grows downward faster than the other one due to the thermodistability, and ruptures. However, the height of the bulge is reduced considerably due to the mean flow. Figure 5.1(c) shows the evolution of the interface and growth in the harmonic modes when $\beta = 30^\circ$. The fundamental mode derives its energy from the mean flow and grows exponentially during initial stages. However, thermodistability begins to interact with surface-wave instability and spreads the energy to the overtones. Overall growth shows that the interface evolves toward a permanent wave form with a sharp front and a gently sloping tail. No capillary waves are observed ahead of the wave. Even in the final period, most of the energy is confined to the fundamental mode and the dominant wavenumber of the equilibrated wave is same as that of the initial disturbance. As we increase the angle of inclination $\beta$ to $60^\circ$ (Fig. 5.1d), growth rate increases and the equilibration is obtained at an earlier time than for $\beta = 30^\circ$. In this case also saturation is observed and the fundamental mode retains most of the energy. However, the mean flow is more efficient in the nonlinear transfer of energy to the superharmonics that saturate with appreciable value. When the plate is vertical (see Fig. 5.1e), surface-wave instability is further enhanced. This causes the crest to travel faster than the trough and steepens the wave front. Thermodistability is also reinforced by the surface-wave instability, and expedites the local thinning. We observe that growth rate of the crest, amplitude of the wave and the wave speed decrease as $\beta$ is increased. In the present study, computed results suggest that when the thermodistability causes the primary instability ($\beta = 0^\circ$), the film always ruptures and when the surface-wave instability is the dominant mechanism ($\beta = 90^\circ$) for wave growth, saturation occurs. For a liquid
draining down an inclined plate, the competition between these two mechanisms determines the fate of the instability.

To illustrate the combined influence of thermocapillarity and surface-wave instability for various disturbances, an extensive parametric study has been performed, and a phase diagram distinguishing the two evolutions, rupture and saturation, is obtained as shown in Fig. 5.2. The parameters of the problem are within the range of long-wave theory. The phase boundary has a steep slope from $\beta=10^\circ$ to $30^\circ$ and approaches monotonically to 0 for $\beta=90^\circ$. This correctly shows that when the film is horizontal, it always ruptures and when it is vertical, it always saturates. To corroborate this statement, in Fig. 5.3, the evolution of a horizontal layer of thin film heated from below is shown. This case is similar to Fig. 5.1 (a) except for the initial disturbance wavenumber $k=0.9k_c, k_M/2$ and $k_M/4$ are used. In all these cases, thermocapillarity overcomes hydrostatic stabilization, and eventually causes rupture. As the wavenumber decreases, the number of fingers increases and suggests that the system has a tendency to choose its own characteristic distance between the fingers. When the plate is vertical (Fig. 5.4), thermocapillary instability is not able to overcome surface-wave instability and the film always equilibrates to a permanent wave form. Extensive numerical experiments suggest that a vertical falling film never ruptures in the range where long-wave theory is valid. It is noticed that in both horizontal and vertical falling films, the amplitude of the wave increase with decrease in wavenumber.

In summary, we note that in the parametric range where the long-wave theory is valid, in a heated horizontal liquid layer ($\beta=0^\circ$) the film always ruptures. On the other hand, in a vertical liquid layer ($\beta=90^\circ$) the film always saturates. For intermediate angles of inclination, rupture occurs for a disturbance with small enough wavenumber.
Figure 5.2: Nonlinear phase diagram: Influence of the wavenumber and the angle of inclination when $C=1$, $S=100$, $M=350$, $Bi=0.1$, and $P=7.0$. The nonlinear phase diagram is obtained from the direct-numerical simulation of the governing equations.
Figure 5.3 (a) $k=0.9 \ k_c$
Final state: Rupture
\[ t_{final}=208.8 \]
\[ h_{min}=0.0099 \]
\[ h_{max}=2.0699 \]

Figure 5.3 (b) $k=k_M/2$
Final state: Rupture
\[ t_{final}=231.6 \]
\[ h_{min}=0.0099 \]
\[ h_{max}=2.6071 \]
Figure 5.3: $G=1$, $S=100$, $P=7$, $M=350$, $Bi=0.1$, $k_M=0.1378$, and $\beta=0^\circ$. The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown for $k=0.9 k_c$, $k_M/2$, and $k_M/4$, respectively, in (a) to (c). In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented.

Modes representation: (---) $n=1$; (---) $n=2$; (- - - -) $n=3$; (.....) $n=4$

Figure 5.4 (a) $k=k_M/2$
Final state: Wavy, but Continuous $t_{final}=651.0$ $h_{min}=0.5562$ $h_{max}=1.9057$
Figure 5.4 (b) $k=k_M/4$
Final state: Wavy, but Continuous

$t_{final}=1014.0$
$h_{min}=0.5469$
$h_{max}=1.8984$

Figure 5.4 (c) $k=k_M/8$
Final state: Wavy, but Continuous

$t_{final}=3084.9$
$h_{min}=0.3992$
$h_{max}=2.2626$
Figure 5.4 (d) $k = k_M/16$
Final state: Wavy, but Continuous
$t_{final} = 2727.6$
$h_{min} = 0.5233$
$h_{max} = 2.0697$

Figure 5.4: $G=1, S=100, P=7, M=350, Bi=0.1, k_M=0.1460$, and $\beta=90^\circ$.
The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown for $k=k_M/2, k_M/4, k_M/8$, and $k_M/16$, respectively, in (a) to (d). In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented.
Modes representation: (---) $n=1$; (-.-.-.) $n=2$; (- - -) $n=3$; (.....) $n=4$

5.4 Merging and Splitting Process

Linear stability analysis of both isothermal and nonisothermal thin-film flows are almost complete and thoroughly understood. However, the nonlinear flow development that ensues the initial exponential growth is still not thoroughly analyzed, especially in heated layers. Figure 5.5 shows a typical linear/nonlinear phase diagram in $(k, G)$ plane for an isothermal film flow. The unstable region is bounded
by an upper neutral curve $k=k_c$ and a lower neutral curve $k=0$ both bifurcating at $G=G_c$ where the subscript "c" denotes critical or cut-off value. For very thin layers, the cut-off wavenumber $k_c$ is very small and hence, the nonlinear dynamics of the system has been studied extensively using long-wave evolution equations (Lin, 1975; Gjevik, 1970; Nakaya, 1975).

In isothermal film flows, the disturbances with wavenumber close to $k_c$ evolve to a sinusoidal wave form. The equilibration to a permanent wave form has been confirmed through the numerical integration of the evolution equation by Pumir, *et al.* (1983) and Joo *et al.* (1991) and from the direct numerical simulation of
Navier-Stokes equations by Chippada et al. (1996). As the wavenumber is decreased, the superharmonics are excited and the wave tends to be broad-banded. This nonlinear transition occurs when $k=k_*=1/2k_c$, and was first studied in detail by Lin (1974). For $k<k_*$, the flow develops sub-critically due to significant nonlinear interplay among the modes. The flow can either saturate to a permanent wave-form or evolve toward a quasi-periodic state. These are discussed in detail by Chippada, et al. (1996). For very small $k$, the flow becomes aperiodic and chaotic. However, in the presence of heat transfer, thermocapillarity interacts with the existing surface-wave instability and can cause rupture.

Figure 5.6 explains how disturbances of different wavelength evolve in a spatially periodic domain when $\beta$, $G$, $Bi$, and $M$ are held constant. The chosen wavenumbers are $k=0.9k_c$, $k_M$, $k_M/2$, $k_M/4$, $k_M/8$, and $k_M/16$, respectively, and $G=1$, $S=100$, $Bi=0.1$, $M=350$, $P=7$ and $\beta=45^\circ$. In all the cases presented, the fundamental mode ($n=1$) grows exponentially during the initial stage as predicted by

---

**Figure 5.6 (a) $k=0.9k_c$**

Final state: Wavy, but Continuous

$t_{final}=325.9$

$h_{min}=0.1537$

$h_{max}=1.7781$
Figure 5.6 (b) $k=k_M$
Final state: Wavy, but Continuous
\[ t_{final}=227.3 \]
\[ h_{min}=0.2491 \]
\[ h_{max}=1.8040 \]

Figure 5.6 (c) $k=k_M/2$
Final state: Wavy, but Continuous
\[ t_{final}=991.6 \]
\[ h_{min}=0.2497 \]
\[ h_{max}=1.8051 \]
Figure 5.6 (d) $k = k_M/4$
Final state: Wavy, but Continuous

$t_{final} = 2038.5$
$h_{min} = 0.4510$
$h_{max} = 1.9922$

Figure 5.6 (e) $k = k_M/8$
Final state: Wavy, but Continuous

$t_{final} = 2458.6$
$h_{min} = 0.4463$
$h_{max} = 2.0956$
the linear theory. When the wavenumber is very close to the cut-off value \( k_c \) (0.9\( k_c \) and \( k_M \)), this mode retains a significant amount of the energy throughout the evolution.

Due to the nonlinear stabilization, all the modes saturate and the interface assumes a finite-amplitude wave form. This wave travels at a constant speed and its shape is almost sinusoidal, corresponding to the "periodic flow" observed by Kapitza & Kapitza (1949). For \( k=k_M \), the equilibrated wave resembles the "single wave" observed by the same researchers.
As we reduce $k$ further, the flow becomes more unstable and the thermocapillarity augments surface-wave instability. The interface no longer maintains single-wave profile. Similar to the observations by Chippada et.al. (1996) in isothermal flows, the number of peaks in the fully saturated state shows dependency on the wavelength of the initial disturbance. This indicates that there is a natural nonlinear wavelength the system chooses to have. In this particular case, the film ruptures only when $k \leq k_M/16$. The amplitude of the wave and hence the wave velocity increases as the wavenumber is decreased. For $k = k_M/8$, the amplitude is as much as twice the base flow thickness in accordance with experimental observations discussed by Lin & Wang (1985).

To analyze the saturation process, the shape of the interface is illustrated in Fig. 5.7, in an increment of 100 nondimensional time units for the simulation shown in Fig. 5.6(e). A domain of three wavelengths is shown for visual clarity. At $t=100$, the free surface still maintains a simple-harmonic shape. As time progresses, surface-wave instability becomes significant and a few lowest superharmonics gain energy. At $t=200$, the interface has a single-wave form. The solitary hump has a sharp leading edge and a gently sloping tail with capillary ripples seen on the interface. At $t=300$, the primary hump splits and subsidiary peaks start growing. These peaks, because of their large amplitude, tend to travel faster than the small amplitude capillary waves and hence, catch up with them as they travel downstream. During this process, the amplitude grows further. However the waves cannot stay merged for a longer time and split further downstream. The merging and splitting of the waves continues to $t=800$, as is evident from the strong nonlinear interaction among the modes (Fig. 5.6e). This process is similar to reorganization of surface waves discussed by Lin & Wang (1985) in the context of a long spatial nonperiodic domain (see Sec.2.2) akin to an actual experimental set-up. The same phenomenon has been
observed previously by Chu & Dukler (1975) in thin liquid film and concurrent gas flow experiments. Beyond this point ($t=800$), all the capillary ripples are consumed by the larger waves and the waves saturate. The surface waves travel at constant speed without any appreciable change in their shape. The plateau between two solitary peaks is of constant thickness and remains calm, free of ripples, while the peaks maintain a constant distance between neighbors. However, spacing itself is not uniform among the crests. Each peak has a sharp front with small capillary ripples,
sometimes called "push waves", traveling ahead of them. They appear traveling on a layer of liquid referred as "lamellar flow" by Stainthorp & Allen (1965).

To summarize, the wavenumber of the disturbance has significant influence on the evolution process. As the wavenumber decreases, nonlinear exchange of energy among the modes becomes critical. Before saturation, the waves reorganize by persistent splitting and merging process. For sufficiently small wavenumbers, the film ruptures.

5.5 Pearson Mode Instability

A thin layer becomes unstable only if is heated from below. At the same time, an unstable layer can be stabilized by cooling from below. Thus the amount of heating and the film thickness, plays an important role in stability control problems. Figure 5.8 shows the effect of film thickness and heating on stability. This is obtained from the linear theory (Kelly, et.al., 1986; Joo, et.al., 1991). The neutral surface is shaped

Figure 5.8: Linear stability diagram: Influence of heating and film thickness (Joo, Davis & Bankoff, 1991).
like a parabola of equal curvature. From this diagram, we infer that for sufficiently thin layers, minimum amount of heating is required to cause instability. Also, for a given heating, increase in the thickness results in stable flow due to the hydrostatic stabilization. This window was first identified by Kelly, *et.al.* (1986) using linear analysis. The critical values of the parameters are (Joo, *et.al.*, 1991):

\[
\left( \frac{Bi \, M}{P} \right)_c = \frac{5}{24} \left( \frac{d + k}{d} \right)^2 \cot^2 \beta \tag{5.3}
\]

\[
G_c \sin \beta = \frac{5 \cot \beta}{2 \frac{d^3}{d^3}} \tag{5.4}
\]

The phase diagram obtained from the linear theory does not give any quantitative information regarding the regime in which rupture occurs. Therefore, using full-scale computation, an extensive parametric search has been done and we show a nonlinear phase diagram in Fig. 5.9 for \( G = 1, S = 100, P = 7, Bi = 0.1, \beta = 45^\circ \) and \( k = k_M \).

In Fig. 5.10, evolution of the interface when \( G = 1, S = 100, P = 7, Bi = 0.1, \beta = 45^\circ \) and \( k = k_M \) at various intensity of heating, \( M = 700, 1050, 1400, \) and 1750, respectively, is shown. As expected, the film ruptures only under sufficient heating \( (M = 1050, 1400, \) and 1750) while saturation occurs when heating is weak \( (M = 700) \). The rupture time decreases with increase in heating. In Fig. 5.11, evolution of the free surface is shown when \( M = 700, P = 7, Bi = 0.1, \beta = 45^\circ \) and \( k = k_M \) for \( G = 0.5, 1.5, \) and 2.5, respectively. Here, we fix the heating and increase the thickness. The film ruptures only when the thickness is sufficiently small \( (G = 0.5) \) while saturation occurs in other cases, *i.e.*, \( G = 1.5 \) and 2.5. The amplitude decreases with the increase in thickness. When \( G \) is large, the instability of Pearson mode appears. The film becomes unstable to disturbances whose wavelengths are comparable to the mean thickness. In these flows, the interaction between the basic temperature field and the perturbation velocity field cause the instability. The convection is dominant
Figure 5.9: Nonlinear phase diagram: Influence of film thickness and heating on rupture dynamics. This diagram is obtained from direct-numerical simulation of governing equations. The other control parameters of the problem are $\mathcal{S} = 100 \ G^{1/3}$, $k=k_M$, $Bi=0.1$, $P=7.0$, and $\beta=45^\circ$. 
Figure 5.10 (a) \( \frac{BiM}{P} = 10 \quad k_M = 0.2012 \)
Final state: Wavy, but Continuous

- \( t_{final} = 137.7 \)
- \( h_{min} = 0.0497 \)
- \( h_{max} = 2.0967 \)

Figure 5.10 (b) \( \frac{BiM}{P} = 15 \quad k_M = 0.2473 \)
Final state: Rupture

- \( t_{final} = 129.4 \)
- \( h_{min} = 0.0099 \)
- \( h_{max} = 2.1330 \)
Figure 5.10 (c) $\frac{BiM}{P}=20$  $k_M=0.2860$
Final state: Rupture $t_{final}=35.18$  $h_{min}=0.0099$  $h_{max}=2.0582$

Figure 5.10 (d) $\frac{BiM}{P}=25$  $k_M=0.3201$
Final state: Rupture $t_{final}=13.41$  $h_{min}=0.0099$  $h_{max}=2.0404$

Figure 5.10: $G=1$, $S=100$, $P=7$, $Bi=0.1$, $k=k_M$, and $\beta=45^\circ$. The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown for $\frac{BiM}{P}=10$, 15, 20, and 25, respectively, in (a) to (d). In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented. Modes representation: (–) $n=1$; (––––) $n=2$; (– - - -) $n=3$; (.....) $n=4$
Figure 5.11 (a) $G=0.5 \quad k_M=0.2268$

Final state: Rupture

$t_{final}=73.09$
$h_{min}=0.0099$
$h_{max}=2.1758$

Figure 5.11 (b) $G=1.5 \quad k_M=0.1876$

Final state: Wavy, but Continuous

$t_{final}=149.1$
$h_{min}=0.1265$
$h_{max}=1.9398$
Figure 5.11 (c) $G=2.5$  \quad $k_M=0.1727$

Final state: Wavy, but Continuous

$t_{final}=100.1$

$h_{min}=0.2265$

$h_{max}=1.5971$

Figure 5.11: $S=G^{\frac{1}{2}}$, $P=7$, $Bi=0.1$, $M=700$, $k=k_M$, and $\beta=45^\circ$. The instantaneous free-surface configuration at $t=0$ (broken line) and at $t=t_{final}$ (solid line) and the corresponding growth in the Fourier modes of the surface wave are shown for $G=0.5$, 1.5, and 2.5, respectively, in (a) to (c). In each figure, the final state of the flow at $t=t_{final}$ and the minimum ($h_{min}$) and maximum ($h_{max}$) local film thickness at that time are also presented.

Modes representation: (—) $n=1$; (¬¬¬) $n=2$; (---) $n=3$; (.....) $n=4$

and supplies energy for the disturbances to grow. The interface stays relatively flat. As discussed in the previous chapter, rupture has not been reported so far for this mode of instability. This indicates that there exists a window of heating intensity for rupture. When the plate is tilted, the liquid drains down due to gravity. This induces surface-wave instability that has the tendency to saturate the flow, leaving a continuous film. As the heating increases, interfacial mode of thermocapillarity
becomes dominant and the film ruptures. However, for very high intensity of heating, the Pearson mode is dominant and the film again stays continuous.

For a given $G$, $M$, $k$ and $\beta$, the thermocapillarity is maximum only when $Bi=1$. For $Bi=0$, the interface is an insulated surface and obtains the temperature of the bottom plate. When $Bi=\infty$, the fluid is highly conductive, and the interface obtains the temperature of the ambient gas. In these extreme cases, thermocapillary instability disappears. We have already shown in Chapter 4 that as $Bi$ is reduced from its critical value of one, rupture time increases significantly. The heat loss is also an important parameter since it influences rupture time significantly.

## 5.6 Concluding Remarks

In the present study, an accurate numerical scheme has been developed, and used in the calculations to understand the influence of combined thermocapillary and surface-wave instabilities in heated thin-film flows. The study shows that the nonlinear dynamics leading to rupture or other waveform is highly dependent on the film thickness, angle of inclination of the plate, intensity of heating, wavenumber of the imposed disturbance and the heat loss at the interface. When the layer is horizontal, the interfacial mode of thermocapillary instability always overcomes the hydrostatic stabilization and causes rupture. When it is vertical, however, rupture disappears in the parametric range considered here, and the film always stays continuous.

The wavenumber plays a significant role in the nonlinear process. If the disturbance wavenumber is close to the cut-off, the interface evolves to a sinusoidal waveform. As the wavenumber is reduced, the waves undergo a merging and splitting process to a saturated state. They become broad-banded and the number of peaks per initial period is determined by the dominant overtone. For small wavenumber and angle of inclination, the layer ruptures. However, increase in the inertial forces
(increase in inclination angle), causes the waves to saturate. The nonlinear interplay between the thermocapillary and surface-wave instabilities decides the final state of the system.

In thin-layers, rupture occurs for a sufficient amount of heating. As the intensity of heating is increased, the Pearson mode becomes dominant due to increased convection inside the layer. This enhances the thermocapillarity by inducing large temperature gradient along the interface. However, rupture does not occur. When the thickness increases, free-surface deformation weakens and the Pearson mode becomes dominant. In this case also, the film stays continuous.
Chapter 6

Rivulet Formation in Three-Dimensional Flows

In this chapter, a mechanism for rivulet formation, shown earlier by Joo, Davis & Bankoff (1996) using the spectral computation of a long-wave evolution equation has been illustrated, for the first time, through full-scale direct numerical simulation of the governing equations. The rivulets form via fingering mechanism similar to what has been observed in a two-dimensional layer. The growth and the orientation of the rivulets are determined by the nonlinear interplay between the surface-wave and the thermocapillary instabilities. Cases are analyzed for two extreme situations; a horizontal layer and a vertical layer. Comparisons with long-wave theory are made to validate the numerical scheme.

6.1 Introduction

A rivulet is a stream of liquid flowing down a solid surface and sharing an interface with a gas. (Young & Davis, 1987). These occur in wide variety of engineering applications such as melting and casting of metals and in condensation process. They play a major role in all these processes since the rivulets have a large surface area to cross-sectional area. Therefore, an understanding of the individual flow regimes will help in the better prediction of heat- and mass-transfer rates.

In a heated layer, the rivulets form by means of a spontaneous rupture, due to the presence of thermocapillary and surface-wave instabilities. They can also form under the influence of external (surface) shear forces. Hence, the mechanism of the
rivulet formation can be well understood by a thorough investigation of the rupture dynamics.

As mentioned before, thin layers become unstable to long surface waves because the shorter waves are suppressed by the capillary effect. Unstable flow may break the film, form dryspots, and make the fluid to go around them. It is also possible that the broken layer will tend to completely rewet the surface over which it was flowing. Hartley & Murgatroyd (1964) studied the conditions under which this happens based on two similar criteria; a dry patch model based on the force balance at the upstream stagnation point, and a rivulet model based on the minimum total energy in a transversely unrestrained stream. They applied the analysis to a vertical laminar layer and to both laminar and turbulent films under the influence of surface-shear stress. Zuber & Staub (1966) extended the model to include the vapor thrust and thermocapillarity, and showed that for liquids of high wettability, the thermal effects become dominant in determining the stability of dry patches. Chung & Bankoff (1980) summarized these studies and generalized the theory to two-component flows to include the effects of non-zero surface-shear stresses.

Young & Davis (1987) studied the mechanism by which the contact lines affect the instabilities in a three-dimensional rivulet flowing down a vertical plane. They used a linear theory to accomplish this. Recently, Schmiki & Laso (1990) conducted experiments in rivulet flows. Though many theories developed in the past on film stability and breakdown, and on problems of determining the minimum flow rate for surface wetting were based on an energetic consideration, only literature available that discusses the mechanism initiating a dry patch is done by Joo, et.al. (1996). They considered a long-wave evolution equation that governs the draining film and through a weakly nonlinear analysis of the truncated system and spectral computation, showed that the coupled thermocapillary and surface-wave instabilities can
create surface deformations that lead to an array of rivulets aligned with the mean flow. Thus, they demonstrated a mechanism for the rivulet formation based solely on the instability mechanism. However, to the author's knowledge, studies that use a full-scale computation to understand this phenomenon is not available in the literature.

In this work, the mechanism suggested by Joo, et.al. (1996) is confirmed through a full-scale simulation for the first time (Krishnamoorthy, Ramaswamy & Joo, 1996a). As mentioned before, with this simulation, we can carry the computations all the way to the formation of a rivulet. In the following section, the method of analysis is discussed. The mechanism for rivulet formation is illustrated for two extreme cases. Results are presented in Sect. 6.3 for a horizontal liquid layer and in Sect. 6.4 for a vertical layer. We discuss the important observations from this study and conclude in Sect. 6.5. Comparison with long-wave theory are made for each case studied.

6.2 Method of Analysis

We select an unstable disturbance based on the linear theory, perturb the free surface and study the temporal evolution of the flow. For this purpose, the linear analysis of long-wave evolution equation is used. The procedure is outlined below (Joo, et.al., 1995):

In a nondimensional Cartesian coordinate system, the evolution equation for a three-dimensional heated layer is expressed as:

\[
\frac{\partial h}{\partial t} + G h^2 \frac{\partial h}{\partial x} \sin \beta + \epsilon \left[ \frac{2G^2}{15} \left( h^2 \frac{\partial h}{\partial x} \right) \sin^2 \beta + \nabla \cdot \left\{ \frac{BiM}{P} \left( \frac{h}{1 + Bi h} \right)^2 \right\} \right] + \frac{G}{3} h^3 \cos \beta \left\{ \nabla h + S \nabla \cdot \left( h^3 \nabla h \right) \right\} + O(\epsilon^2) = 0, \tag{6.1}
\]
where $h(x,y,t)$ is the film thickness, $x$ and $y$ are the streamwise and spanwise coordinates, and $t$ is the time. Here, $\nabla = (\partial/\partial x, \partial/\partial y)$. A linear stability analysis of this equation can be carried out by considering an infinitesimal harmonic disturbance of the form,

$$
h = 1 + \delta e^{i(kx-\Gamma t)}
$$

where, $0 \leq \delta \ll 1$, the wavenumber vector $\vec{k} = k(\cos \theta, \sin \theta)$, complex frequency $\Gamma = \Gamma_R + i\Gamma_I$, and the subscripts $R$ and $i$ denote real and imaginary parts, respectively. Here, $\theta$ is the oblique angle which is zero for a two-dimensional (transverse) wave and $\pi/2$ for a pure longitudinal wave. Substituting the above expression in Eq. 6.1 and linearize it, we obtain

$$
\Gamma_i = c = G \sin \beta, \quad (6.3)
$$

$$
\Gamma_R = \epsilon k^2 \left( \frac{2G^2}{15} \cos^2 \theta \sin^2 \beta + \frac{BiM}{P} \frac{1}{(1 + Bi)^2} - \frac{G}{3} \cos \beta - S k^2 \right) \quad (6.4)
$$

where $\Gamma_i$ is the phase speed and $\Gamma_R$ is the growth rate. The cut-off wavenumber $k_c$ can be obtained by setting $\Gamma_R = 0$, or

$$
k_c = \left\{ \frac{1}{S} \left[ \frac{2G^2}{15} \cos^2 \theta \sin^2 \beta + \frac{BiM}{P} \frac{1}{(1 + Bi)^2} - \frac{G}{3} \cos \beta \right] \right\}^{\frac{1}{2}} \quad (6.5)
$$

We solve an initial value problem by imposing a simple-harmonic disturbance of the form

$$
h(x,y,0) = 1 + 0.1 \cos(k_x x) + 0.1 \cos(k_y y) \quad (6.6)
$$

where $k_x$ and $k_y$ are respectively the streamwise and the spanwise wavenumber of the disturbance such that $\vec{k} = \sqrt{k_x^2 + k_y^2}$, and $k_x = k \cos \theta$ and $k_y = k \sin \theta$ and $\vec{k} < k_c$. We integrate three-dimensional governing equations, Eqs. 3.17 to 3.21, along with the boundary conditions (Eqs. 2.10, 2.15, 2.23 and 2.24), and examine the temporal evolution of the free surface. The analysis will be done on one spatial
period \((2\pi/k_x, 2\pi/k_y)\). The growth of subharmonics, that can occur normally in a laboratory situation, is not allowed.

We stop the computation at any moment when the local film thickness becomes less than 0.01 and assume rupture at that spot. Beyond this point intermolecular forces will become significant and the governing system will be insufficient for the accurate description of the ensuing flow.

The computational domain is discretized into non-overlapping four-node linear-tetrahedral elements. The results are presented with instantaneous free-surface configuration, \(z=h(x,y,t)\), and contour plots of the surface elevation at various time levels, and the norms \(N_x\) and \(N_y\), which measure, respectively, the streamwise and spanwise components of the total wave energy:

\[
N_x(t) = \frac{k_y}{2\pi} \int_0^{2\pi/k_y} \left( \sum_{n=1}^{N} a_n^2 \right)^{\frac{1}{2}} \, dy,
\]

(6.7)

\[
N_y(t) = \frac{k_x}{2\pi} \int_0^{2\pi/k_x} \left( \sum_{m=1}^{M} b_n^2 \right)^{\frac{1}{2}} \, dx,
\]

(6.8)

where the Fourier spectra \(a_n\) and \(b_n\) are

\[
h(x,y,t) = \sum_{n=0}^{N} a_n(y,t) e^{i k_x x} = \sum_{m=0}^{M} b_m(x,t) e^{i k_y y},
\]

(6.9)

and \(2N\) and \(2M\) are the total number of grid points in the streamwise and the spanwise directions, respectively.

### 6.3 Horizontal Film

When the layer is horizontal, there is no mean flow. The thermocapillarity is the primary instability mechanism. It has to overcome the stabilizing effects of hydrostatic and capillary effects. In Fig. 6.1, the evolution of the layer is shown when
Figure 6.1 (a)
Full-Scale Computation
(Finite-Element Method)
\[ t=0.0 \]
\[ h_{\text{min}}=0.80 \]
\[ h_{\text{max}}=1.20 \]

Figure 6.1 (b)
Spectral Computation of
Long-Wave Evolution Equation
\[ t=0.0 \]
\[ h_{\text{min}}=0.80 \]
\[ h_{\text{max}}=1.20 \]

Horizontal Layer
Figure 6.1 (c)  
Full-Scale Computation  
(Finite-Element Method)  
$t = 500.0$  
$h_{min} = 0.5520$  
$h_{max} = 1.3930$

Figure 6.1 (d)  
Spectral Computation of  
Long-Wave Evolution Equation  
$t = 500.0$  
$h_{min} = 0.5448$  
$h_{max} = 1.3911$

Horizontal Layer
Figure 6.1 (e)
Full-Scale Computation
(Finite-Element Method)
\( t=800.0 \)
\( h_{\text{min}}=0.4043 \)
\( h_{\text{max}}=1.5931 \)

Figure 6.1 (f)
Spectral Computation of
Long-Wave Evolution Equation
\( t=800.0 \)
\( h_{\text{min}}=0.4027 \)
\( h_{\text{max}}=1.5880 \)

Horizontal Layer
Figure 6.1 (g)
Full-Scale Computation
(Finite-Element Method)
\( t=1000.0 \)
\( h_{\text{min}}=0.2369 \)
\( h_{\text{max}}=1.8259 \)

Figure 6.1 (h)
Spectral Computation of
Long-Wave Evolution Equation
\( t=1000.0 \)
\( h_{\text{min}}=0.2461 \)
\( h_{\text{max}}=1.8176 \)

Horizontal Layer
Figure 6.1 (i)  
Full-Scale Computation  
(Finite-Element Method)  
\[ t=1180.0 \]
\[ h_{\text{min}}=0.0983 \]
\[ h_{\text{max}}=2.2101 \]

Figure 6.1 (j)  
Spectral Computation of  
Long-Wave Evolution Equation  
\[ t=1163.5 \]
\[ h_{\text{min}}=0.1012 \]
\[ h_{\text{max}}=6.9425 \]

Horizontal Layer
Figure 6.1: $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_x=0.05$, $k_y=0.05$, and $\beta=0^\circ$. The free-surface shape and contour plot of surface elevation obtained using full-scale computation (FEM) and spectral computation of long-wave evolution equation are shown at various time levels. At $t=1242$, the long-wave theory is no longer valid and only results from the full-scale computation are plotted.

$G=1$, $S=100$, $Bi=1$, $M=35.1$, $P=7.02$, $k_x=0.05$ and $k_y=0.05$. In this figure, the instantaneous free-surface configuration and the contour plot of the surface elevation are shown at various times. The results from both full-scale computation and spectral computation of long-wave evolution equations are shown simultaneously for comparison.

Figures 6.1(a) and (b) show the shape at $t=0$. Since $k_x=k_y$, the initial perturbation is symmetric. The trough lies in the center of the domain surrounded by
the crests at the four corners. Since the trough lies closer to the bottom plate that is hotter than the surrounding fluid, the thermocapillarity sets in and displaces the fluid from the hotter trough to the colder crests. As a result, the trough is drawn downward while the crests begin growing upwards. This is shown in Fig. 6.1(c), where at $t=500$, the crests have grown to 140% of their initial thickness while the trough has thinned almost by 30%. As the trough gets hotter and hotter, thermocapillarity is enhanced and the downward growing trough manifests itself as a finger. The spectral simulation of long-wave evolution equation (Fig. 6.1d) also predicts the same. As the trough thins further, it feels the bottom. The plate offers the resistance due to the viscous effects of the fluid. Consequently, the edge becomes flat. However, it has a sharp corner, and is subjected to high capillary pressure. At the same time, thermocapillarity induces flow toward the plate. Hence, the fluid trapped at the center of the annulus is pushed upward to conserve the mass. This sequence of events is evident from Figs. 6.1(e) and (g). The corresponding states from long-wave computations are shown in Figs. 6.1(f) and (h). Since the mean flow is absent and the imposed disturbance is symmetric, there is no preferred direction for the growth and the finger grows symmetrically. We observe a three-dimensional fingering process whose mechanism is similar to a two-dimensional fingering process shown in Fig. 4.6. At $t=1150$, the inertial effects become so dominant that the evolution equation ceases to follow the nonlinear dynamics thereafter (Fig. 6.1j). The downward growing finger continues to evolve and finally, at $t=1242$, touches the plate forming a concave-dome shaped rivulet as shown in Fig. 6.1(k). This justifies the use of full-scale computation. However, the spectral computation of long-wave evolution equation and the full-scale computation agree very well over a long period of evolution.
In Fig. 6.2, the growth of wave energy in the streamwise and spanwise directions is shown. From this figure, it is very obvious that there is no nonlinear saturation and the energy of the system increases until the film breaks. Also, \( N_x = N_y \), because \( k_x = k_y \). Our solutions compare very well with the long-wave theory till \( t = 1000 \), after which higher harmonics gain significant amount of energy and the long-wave theory fails to follow the dynamics.

In this particular problem, an axisymmetric rivulet has formed because \( k_z = k_y \). A three-dimensional disturbance may be considered as two waves of lower order in the streamwise and the spanwise directions characterized by the wavenumbers \( k_x \) and \( k_y \), respectively. The nonlinear interplay between these waves results in different rivulet patterns depending on the wavenumbers.

**Figure 6.2 (a)**
Full-Scale Computation
(Finite-Element Method)

**Figure 6.2 (b)**
Spectral Computation of
Long-Wave Evolution Equation

**Figure 6.2:** \( G=1, S=100, B_i=1, M=35, P=7, k_x=0.05, k_y=0.05 \), and \( \beta=0^\circ \). The energy norms \( N_x \) (---), in the streamwise direction, and \( N_y \) (-----), in the spanwise direction, are compared.
6.4 Vertical Film

When the film is vertical, the flow is driven by gravity. In this case, the thermocapillary and surface-wave instabilities enhance each other and the film may saturate and stay continuous or rupture depending on which mode of instability is dominant. In our simulations, the plane is inclined only in the streamwise direction. Consequently, there will not be any mean flow in the spanwise direction and the surface-wave instability will not appear in that direction.

In Fig. 6.3, the evolution of a vertical film is shown when \( G=1, S=100, Bi=1, M=35, P=7, k_x=0.05, \) and \( k_y=0.05 \). The instantaneous free-surface configuration and the contour plot of the surface elevation obtained using the full-scale computation and the spectral computation of long-wave evolution equation are shown at various time levels. Figure 6.3(a) shows the shape at \( t=0 \). Since \( k_x=k_y \), the initial perturbation is symmetric. The trough lies in the center of the domain surrounded by the crests at the four corners. Since the trough lies closer to the bottom plate which is hotter than the surrounding fluid, the thermocapillarity sets in and displaces the fluid from the hotter trough to the colder crests. During the initial period, as the liquid drains downward, the surface-wave instability dominates and the flow evolves downstream as shown in Figs. 6.3(c) and (d). Here the local phase speed of the layer is proportional to its thickness as per linear theory. As time progresses, the thinning of the liquid layer persists (Figs. 6.3e and f) and the thermocapillarity begins to dictate the growth of the layer. Without mean flow in the spanwise direction, the liquid is displaced laterally due to thermocapillarity. This process is similar to the evolution of a heated thin film on a horizontal substrate. The thin-layer effect causes the fingers to appear and a three-dimensional longitudinal pattern (rivulet) develops along the centerline of the stream. This sequence of events is evident from Figs. 6.3(g) to (j). At \( t=975 \), (Figs. 6.3k and l), all the superharmonics are excited.
Figure 6.3 (a)
Full-Scale Computation
(Finite-Element Method)
\[ t=0.0 \]
\[ h_{\text{min}}=0.80 \]
\[ h_{\text{max}}=1.20 \]

Figure 6.3 (b)
Spectral Computation of
Long-Wave Evolution Equation
\[ t=0.0 \]
\[ h_{\text{min}}=0.80 \]
\[ h_{\text{max}}=1.20 \]

Vertical Layer
Figure 6.3 (c)
Full-Scale Computation
(Finite-Element Method)
\( t=150.0 \)
\( h_{\text{min}}=0.6643 \)
\( h_{\text{max}}=1.3754 \)

Figure 6.3 (d)
Spectral Computation of
Long-Wave Evolution Equation
\( t=150.0 \)
\( h_{\text{min}}=0.6601 \)
\( h_{\text{max}}=1.3813 \)

Vertical Layer
Figure 6.3 (e)
Full-Scale Computation
(Finite-Element Method)
\( t=300.0 \)
\( h_{\text{min}}=0.5933 \)
\( h_{\text{max}}=1.3741 \)

Figure 6.3 (f)
Spectral Computation of
Long-Wave Evolution Equation
\( t=300.0 \)
\( h_{\text{min}}=0.5820 \)
\( h_{\text{max}}=1.3663 \)

Vertical Layer
Figure 6.3 (g)
Full-Scale Computation
(Finite-Element Method)
\[ t = 600.0 \]
\[ h_{\text{min}} = 0.5238 \]
\[ h_{\text{max}} = 1.5674 \]

Figure 6.3 (h)
Spectral Computation of
Long-Wave Evolution Equation
\[ t = 600.0 \]
\[ h_{\text{min}} = 0.5146 \]
\[ h_{\text{max}} = 1.5586 \]

Vertical Layer
Figure 6.3 (i)
Full-Scale Computation
(Finite-Element Method)
\[t=900.0\]
\[h_{\text{min}}=0.2490\]
\[h_{\text{max}}=2.0336\]

Figure 6.3 (j)
Spectral Computation of
Long-Wave Evolution Equation
\[t=900.0\]
\[h_{\text{min}}=0.3135\]
\[h_{\text{max}}=2.0422\]

Vertical Layer
Figure 6.3 (k)
Full-Scale Computation
(Finite-Element Method)
\( t = 975.0 \)
\( h_{\text{min}} = 0.1212 \)
\( h_{\text{max}} = 2.2219 \)

Figure 6.3 (l)
Spectral Computation of
Long-Wave Evolution Equation
\( t = 974.2 \)
\( h_{\text{min}} = 0.2104 \)
\( h_{\text{max}} = 4.5278 \)

Vertical Layer
Figure 6.3: $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_x=0.05$, $k_y=0.05$, and $\beta=90^\circ$. The free-surface shape and contour plot of surface elevation obtained using full-scale computation (FEM) and spectral computation of long-wave evolution equation are shown at various time levels. At $t=1027$, the long-wave theory is no longer valid and only results from the full-scale computation are plotted.

by this nonlinear process and the long-wave theory is no longer valid beyond this time. However, using full-scale computation, we can integrate the governing system all the way to rupture. The final state, $t=1027$, is shown in Fig. 6.3(m). This simulation confirms the observation by Joo et al. (1996) that in a vertical layer, the longitudinal rivulets aligned with the mean flow can form only when both the thermocapillary and surface-wave instabilities are properly balanced and neither of these two instabilities alone has the tendency to develop such pattern. This
simulation also explains a mechanism for rivulet formation purely from a stability point of view.

The energy norm of the free-surface evolution is shown in Fig. 6.4. In this simulation also, we observe that the long-wave theory agrees very well with the full-scale computation up to $t=800$, after which it fails to follow the dynamics of the flow. The energy along the streamwise direction ($N_x$) saturates in both the cases which indicates the formation of longitudinal rivulets aligned with the mean flow.

In Figs. 6.5(a) to (c), the evolution of the thin film is shown for various time levels indicated when the spanwise wavenumber $k_y=0.25$. All other parameters are identical to the previous case. In this case local thinning rates are smaller and hence, the rupture time is increased. However, fingering occurs in an early stage of the evolution and the rivulets are much larger than the previous case.

![Figure 6.4(a) FEM](image1)

![Figure 6.4(b) Long-wave Theory](image2)

**Figure 6.4:** $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_z=0.05$, $k_y=0.05$, and $\beta=90^\circ$. The energy norms $N_x$ (—), in the streamwise direction, and $N_y$ (-.-.), in the spanwise direction, are compared.
Figure 6.5 (a)
\[ t=0.0 \\
\ h_{\text{min}}=0.80 \\
\ h_{\text{max}}=1.20 \]

Figure 6.5 (b)
\[ t=500.0 \\
\ h_{\text{min}}=0.6563 \\
\ h_{\text{max}}=1.3610 \]

Full-Scale Computation (Finite-Element Method)
Vertical Layer
Figure 6.5: $G=1$, $S=100$, $Bi=1$, $M=35$, $P=7$, $k_x=0.05$, $k_y=0.025$, and $\beta=90^\circ$. The free-surface shape and contour plot of surface elevation obtained using full-scale computation (FEM) are shown at various time levels. The film ruptures at $t=1900$. 

Figure 6.5 (c) $t=1200.0$ $h_{\text{min}}=0.5066$ $h_{\text{max}}=1.5030$ 

Figure 6.5 (d) $t=1900.3$ $h_{\text{min}}=0.0099$ $h_{\text{max}}=2.2676$
6.5 Concluding Remarks

The rupture is the underlying mechanism in the formation of drypatches and rivulets. The numerical experiments show that in a horizontal layer, spherical rivulets form via fingering mechanism similar to what has been observed in a two-dimensional layer. The formation is axisymmetric if the streamwise and spanwise wavenumbers are equal i.e., the imposed disturbance is axisymmetric.

When the layer is kept vertical, there is a mean flow in the streamwise direction only. This induces surface-wave instability. This instability coupled with the thermocapillarity causes the formation of longitudinal rolls aligned with the mean flow. The shape and size of the rivulets highly depend on the wavenumber of the imposed disturbance. In all the simulations, we observe that the long-wave theory agrees very well with the full-scale computation over a long period of evolution. However, near rupture inertial effects become significant, and this theory fails to follow the dynamics of the flow.
Chapter 7

General Conclusions

7.1 Conclusion

An accurate and efficient three-dimensional numerical procedure, using the finite-element method has been developed to study the instabilities in a heated falling film. The computational efficiency is achieved by:

1. Employing the ALE procedure which allows us to handle the moving boundary without causing severe mesh distortion;

2. Using the Chorin-type time splitting algorithm which decouples pressure from the velocity field, thereby allowing us to implement fast iterative solvers.

The comparison of the numerical results with the benchmark solutions establishes the accuracy of the numerical scheme. Computations have been done using CRAY-YMP and SPARC-10 machines.

An extensive numerical study has been conducted on both two- and three-dimensional layers in a spatially periodic domain. The numerical experiments show that in a horizontal layer, when the interfacial mode of thermocapillarity is significant, the film always ruptures via a fingering mechanism associated with the lubrication pressure. In a vertical layer, though this mode of instability is enhanced by the surface-wave instability, the film always stays continuous in the parametric range where long-wave theory is valid. For intermediate angles of inclination, rupture occurs for a disturbance with small enough wavenumber.
In a horizontal layer, the Pearson mode of thermocapillarity is dominant at very high intensity of heating, or in thick films. In this case, the film always stays continuous. This indicates that there exists of a window of heating intensity for rupture. When the plate is tilted, the liquid drains down due to gravity. At low intensity of heating, the surface-wave instability is the primary instability mechanism and the film stays continuous. As the heating increases, interfacial mode of thermocapillarity becomes dominant and the film ruptures. However, at very high intensity of heating, the Pearson mode is dominant and the film again stays continuous.

To illustrate the combined influence of thermocapillarity and surface-wave instability for various disturbances, an extensive parametric study has been performed, and a phase diagram distinguishing the two evolutions, ruptured film and wavy but continuous film, is presented. The wavenumber plays a significant role in the nonlinear process. If the disturbance wavenumber is close to the cut-off, the interface evolves to a sinusoidal waveform. As the wavenumber is reduced, the waves undergo a merging and splitting process to a saturated state. They become broad-banded and the number of peaks per initial period is determined by the dominant overtone. For small wavenumber and angle of inclination, the layer ruptures.

Spontaneous rupture is the underlying mechanism in the formation of dry-patches and rivulets. Three-dimensional simulations show that in a horizontal layer, spherical rivulets form by a three-dimensional fingering mechanism similar to what has been observed in a two-dimensional layer. When the layer is kept vertical, there is a mean flow in the streamwise direction inducing the surface-wave instability. This coupled with the interfacial mode of thermocapillarity in the spanwise direction, leads to the formation of longitudinal rolls aligned with the mean flow. In all the cases, the shape and size of the rivulets highly depend on the wavenumber of the imposed disturbance.
7.2 Future Work

Some of the possible future works are listed below:

1. Since in the present work, a powerful three-dimensional numerical procedure has been developed, several problems of practical interest can be readily simulated with simple modifications.

2. Our model does not include the effects of molecular forces, evaporation losses, and surface contamination. Incorporating these effects is rather straightforward. It will be interesting to study how the layer evolves under the combined influence all the instabilities discussed so far.

3. In an isothermal flow, it is well known that the instabilities are of convective nature. However, the nature of the instability in a non-isothermal flow is still an open question.

4. When a layer breaks and forms rivulets, it creates drypatches and the liquid goes around them. If the liquid is non-volatile, the mean flow may tend to rewet the surface, drypatches may disappear and flow can become uniform again. Dynamics in this case involve establishing contact lines, with a corresponding contact angle. It is a challenging problem to simulate the transition involved in this process.

5. Finally, examining the influence of electrostatic and magnetic fields in thin-film instability is another area where very few numerical studies have been done so far.
VIDEO COPY OF THE NUMERICAL SIMULATIONS IS AVAILABLE
FROM THE AUTHOR UPON REQUEST
Bibliography


