THE NUMERICAL SIMULATION OF NON-ISOTHERMAL THIN LIQUID FILM FLOW ON INCLINED PLANE

BY

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ABSTRACT

The classical problem of the stability and dynamics of thin liquid films on solid surfaces has been studied extensively. Particularly, thin liquid films subjected to various physico-chemical effects such as thermocapillarity, solutal-Marangoni and evaporative instabilities at the film surface has been the focus of research for more than two decades. Various flow configurations of thin film such as thin film on plane, inclined, and wavy surfaces had been the subject of recent investigations.. An inclined film compared to a horizontal film, also experiences the gravity force which may significantly influence the nonlinear dynamics of the film coupled with other forces. In this research, an attempt is made to characterise qualitatively the stability and dynamics of a thin liquid film on an inclined plane which is subjected to instabilities owing to thermocapillarity and evaporative effects as well as van der Waals attractive intermolecular forces, and to compare the results to those in the standard literature. For a Newtonian liquid, flow in thin liquid film on a planar support and bounded by a passive gas, is represented by Navier-Stokes equation, equation of continuity and appropriate boundary conditions. The external effects are incorporated in the body force term of the Navier-Stokes equation. These governing equations are simplified using the so called long-wave approximation to arrive at a nonlinear partial differential equation, henceforth called equation of evolution (EOE), which describes the time evolution of the interfacial instability in the film caused by internal and/or external effects. Efficient numerical method is required for the solution of the equation of evolution (EOE) in order to comprehend the nonlinear dynamics of the thin film. Here we present the results of our numerical simulations using Crank-Nicholson implicit finite difference scheme applied to the thin film model incorporating instabilities owing to gravity, evaporation and thermo-capillarity. Comparison of our results with those obtained from Spectral method, show remarkable agreement for most of the cases investigated. The film rupture times obtained using our implicit finite difference method closely conform to those of Fourier spectral results of Joo et al. (1991) within a deviation of 1.5% for films going to rupture. For cases not resulting into rupture, the film interface profiles at various stages of deformation are almost identically similar to the profiles obtained in our numerical simulations. Thus implicit Crank-Nicholson mid-point rule proves to be an efficient and reliable method for numerical simulation of the nonlinear dynamics of thin film flows.

Keywords: *Thin liquid film flow; Nonlinear Dynamics; Implicit Finite Difference; Spectral Method*.

خلاصة البحث

الدراسة الكلاسيكية لمشكلة إستقرار وديناميكية الطبقات الرقيقة للسوائل على الأسطح الصلبة تمت على نطاق واسع من قبل.بالاخص، استعمال تعريض الطبقات الرقيقة للسوائل لمختلف الآثار الفيزيائية والكيميائية مثل الترموكابلريتي ،محاليل مارانجوني وعدم إستقرار التبخر على سطح الغشاء الذي تركزت عليه البحوث لأكثر من عقدين من الزمن.والموضوع الذي يتركز عليه البحث حاليا هو تركيب الطبقات الرقيقة للسوائل مثل طبقة رقيقة على مستوي ، مائل ، الأسطح المتموجة.بالمقارنة بين الأغشية الأفقية والمائلة، وكذا تجريب تأثير قوة الجاذبية الكبيرعلى الدينامية غير الخطية للأغشيةعلى قوى أخرى. في هذا البحث، ونحن نحاول دراسة إستقرار وديناميكية الطبقات الرقيقة للسوائل المعرضة للترموكابيلري والتبخر الغيرمستقر على السطح الحر إلى جانب عدم الاستقرار بسبب تأثيرجاذبية فان دير فال ، وذلك باستخدام المحاكاة العددية.بالنسبة لسائل النيوتونية، التدفق في الطبقات الرقيقة للسوائل على دعم مستو ويمحدودة بالغاز السلبي، الممثل بمعادلة نافيير ستوكس ، معادلة الاستمرارية وشروط الحدود المناسبة.تندرج الآثار الخارجية على مدى قوة الجسم منمعادلة نافيير ستوكس.يتم تبسيط هذه المعادلات التي تعتمد على استخدام ما يسمى تقريب الموجة الطويلة للوصول إلى المعادلة التفاضلية الجزئية غير الخطية، والتي تدعى معادلة التطور (EOE).الذي يصف تطور الزمن من عدم الاستقرار بينية في الطبقات الرقيقة للسوائل الناجمة عن تأثيرات داخلية / أو خارجية. مطلوب طريقة عددية فعالة من أجل إيجاد حلول معادلة التطور (EOE) من أجل فهم ديناميكيات غير الخطية للطبقات الرقيقة للسوائل.هنا نقدم نتائج المحاكاة العددية التي تحصلنا عليها باستخدام مخطط كرانك-نيكلسون الضمني محدود الفرق مخطط وتطبيقه على نموذج من الطبقات الرقيقة للسوائل التي تتضمن عدم الاستقرار بسبب الجاذبية، والتبخير والحرارية الشعرية. مقارنة نتائجنا مع تلك التي تم الحصول عليها من إستعمال طريقة الطيفي، تظهر اتفاق ملحوظا في معظم الحالات التي حققت فيها.

APPROVAL PAGE

I certify that I have supervised and read this study and that in my opinion, it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Science in Mechanical Engineering.

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DECLARATION

I hereby declare that this dissertation is the result of my own investigations, except where otherwise stated. I also declare that it has not been previously or concurrently submitted as a whole for any other degrees at IIUM or other institutions.

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Firstly, it is my utmost pleasure to dedicate this work to my dear parents and my family, who granted me the gift of their unwavering belief in my ability to accomplish this goal: thank you for your support and patience.

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TABLE OF CONTENTS

LIST OF SYMBOLS and ABBREVIATIONS

A = Non dimensional Hamaker constant

D = Ratio of vapour to liquid density

E = Evaporation number

G = Non dimensional gravitational number,

M = Marangoni number

S = Non dimensional mean surface tension

P = Prandtl number

Re = Reynolds Number

Abbreviations

FD = Finite difference

Greek Symbols

γ = surface tension gradient

ρ = density

κ = thermal diffusivity

σ = surface tension

μ = dynamic viscosity

ν = kinematic viscosity

φ = Van der Waals potential function

LIST OF FIGURES

Figure 5	Evolution of free surface configurations with surface wave and thermocapi-llarity instability when k=0.7, and G = 5, $\beta = 45^0$, $\Delta\tau$=0.5, $0 \le \tau \le 1.6$, KM/P=1, K = 0.1, $\overline{S}$=0.1, $\overline{E}$=0, E^2/D=0. Red colour shows the last profile at τ = 1.6.
Figure 6	Evolution of film instability leading to film rupture for an evaporating layer shown with $\Delta\tau$ = 0.05, and k = 0.7, G=0, KM/P=0.01, $\overline{E}$=0.1, K=0.1, P=1, and $\overline{S}$=0.1. Rupture time τ_R for spectral method (Joo et al. 1991) is 4.9388, and τ_R for implicit FDM is 4.8915 for the above parameter values. Deviation is 0.96%. Red colour shows the surface configuration at the point of rupture.
Figure 7a	Film interface evolution for evaporating horizontal layers in the presence of vapour recoil for k=0.5. Free surface profiles are shown for time increment $\Delta\tau$=0.05. Parameter values are: G=0, $\overline{E}$=0.1, K=0.1, $\overline{S}$=0.1, P=1, E^2/D=2, D=0.0002. Rupture time, τ_R from FD simulation is 4.6530 which is closely conforms to τ_R=4.6425 (Spectral method). Deviation is 0.23%.
Figure 7b	Film interface evolution for evaporating horizontal layers in the presence of vapour recoil for k=0.7. Free surface profiles are shown for time increment $\Delta\tau$=0.05. Parameter values are: G=0, $\overline{E}$=0.1, K=0.1, $\overline{S}$=0.1, P=1, E^2/D=2, D=0.0002. Rupture time, τ_R from FD simulation is 4.4150 which closely agrees with τ_R=4.3475 from the spectral method. Deviation is 1.55%.
Figure 7c	Evolution of the film interface for evaporating horizontal layers in the presence of vapour recoil for k=1.0. Free surface profiles are shown for time increment $\Delta\tau$=0.05. Parameter values are: $\overline{E}$=0.1, K=0.1, $\overline{S}$=0.1, P=1, E^2/D=2, G=0. Rupture time, τ_R from FD simulation is 3.1404 whereas spectral method simulation show no rupture until τ=3.15.
Figure 8	Free surface profiles for an evaporating horizontal layer with thermocapilla-rity leading to rupture for k=0.5, G=0, D=0.0005, $\overline{E}$=0.1, K=0.1, $\overline{S}$=0.1, P=1, KM/P=2, M=20, and $\Delta\tau$=0.05. Film profiles are shown culminating to rupture at τ_R= 4.5940. Rupture time τ_R (for **s**pectral method) = 4.5894. Deviation is less than 0.1%.
Figure 9a	Figure 9a: Free surface profiles for evaporating layers with gravitational effects leading to rupture for $\beta=0^0$. Parameters are: k=0.7, $\overline{E}$=0.1, K=0.1, P=1, $\overline{S}$=0.1, G=5, E^2/D=0.0005, KM/P=0.1, M=1, with $\Delta\tau$=0.05. Rupture time from FD simulations is 5.1480.

τ_R (from spectral method) = 5.1769. Deviation is 0.56%.

Figure 9b	Free surface profiles for evaporating layers with gravitational effects leading to rupture for β=15^0. Parameters are: k=0.7, $\bar{\bar{E}}$=0.1, K=0.1, P=1, $\bar{\bar{S}}$=0.1, G=5, E^2/D=0.0005, KM/P=0.1, M=1, with Δτ=0.05. Rupture time from FD simulations is 5.1290. τ_R (from spectral method) = 5.1525. Deviation is 0.46%.
Figure 9c	Free surface profiles for evaporating layers with gravitational effects leading to rupture for β=30^0. Parameters are: k=0.7, $\bar{\bar{E}}$=0.1, K=0.1, P=1, $\bar{\bar{S}}$=0.1, G=5, E^2/D=0.0005, KM/P=0.1, M=1, with Δτ=0.05. Rupture time τ_R from FD simulations is 5.0730. τ_R (from spectral method) = 5.0687. Deviation is 0.085%.
Figure 9d	Free surface profiles for evaporating layers with gravitational effects leading to rupture for β=45^0. Parameters are: k=0.7, $\bar{\bar{E}}$=0.1, K=0.1, P=1, $\bar{\bar{S}}$=0.1, G=5, E^2/D=0.0005, KM/P=0.1, M=1, with Δτ=0.05. Evolution of surface profiles are shown upto τ = 4.3, and are almost identical in the two cases.

LIST OF TABLES

CHAPTER ONE

INTRODUCTION

1.1 BACKGROUND OF THE STUDY

Thin liquid films are ubiquitous entities in a variety of settings. A liquid film maybe considered thin if its thickness is much smaller than its lateral dimensions. In geology, they appear as gravity currents under water or as lava flows (Huppert and Simpson, 1980; Huppert, 1982a). In engineering, thin films serve in heat and mass transfer processes to limit fluxes and to protect surfaces, and applications arise in paints, adhesives, and membranes. Thin liquid films display a variety of interesting dynamic characteristics. Because the interface between the thin film layer and the atmosphere is deformable, thin films can develop wave motion. The interfacial waves in a thin film propagating flowing down an inclined plane display fascinating nonlinear phenomena such as complex disordered patterns, solitary waves and transverse secondary instabilities. The film can rupture, leading to holes in the liquid that expose the surface to the atmosphere. The thin film flows are governed to a good approximation by the equations of motion simplified in the long wave (lubrication) approximation.

1.2 STATEMENT OF THE PROBLEM

In the case of Newtonian fluid flow of thin liquid film on a solid support and bounded by a passive gas, the dynamics are represented by Navier Stokes equations and equation of evolution together with appropriate boundary conditions. The external effects are generally incorporated in the body force term of the Navier Stokes equations. These governing equations can then be simplified using the so called long wave approximation to arrive at fourth order nonlinear partial differential equation, henceforth called the equation of evolution which describes the time evolution of the interfacial instability caused by internal and/or external effects. The details of the derivation of the equation of evolution are available in the literature (Williams & Davis, 1982; Burelbach et al., 1988: Joo et al., 1991).

1.3 PURPOSE OF THE STUDY

The stability and dynamics of thin liquid films on solid substrates has been studied extensively for the past three decades. Particular attention has been focused on the case of thin liquid films subjected to various physical-chemical effects such as thermocapillarity, solutal Marangoni and evaporative instabilities at the surface. Furthermore, if the film is inclined at an angle to the horizontal, it experiences the gravitational force which might influence the nonlinear dynamics of the film coupled to other forces. Heat transfer in thin liquid film flow on an inclined plane occurs in numerous chemical and biochemical processes such as solid coating, food processing and in systems with evaporative cooling as well as high throughput exchange devices. The understanding of stability, dynamics and morphology of supported thin (<100nm) liquid films are important in phenomena like flotation, adhesion of fluid particles to surfaces, kinetics and thermodynamics of precursor films in wetting heterogeneous nucleation, film boiling/condensation, multilayer adsorption/film pressure, instability of biological films/membranes, and many other areas (Gaines, 1966; Bikerman, 1973; Sharma and Ruckenstein, 1986a; Grotberg, 1994; Wong *et al.*, 1996).

1.4 RESEARCH OBJECTIVES

The main goal of this research is to characterize the flow of a thin liquid film layer on an inclined plane which is subjected to evaporative and thermocapillarity instabilities as well instabilities due to Van Der Waals forces using numerical simulations and to study the stability and rupture of the thin liquid film layer. The specific objectives are:

1- To model the non-isothermal flow of a Newtonian thin liquid film down an inclined plane subjected to instabilities owing to evaporative and thermocapillarity and van der Waals interactions using equations of motion and continuity equation and associated boundary conditions.
2- To derive a nonlinear equation of evolution (EOE) for the film interface describing the dynamics of the inclined thin film flow subjected to various physico-chemical effects.
3- To solve the nonlinear equation of evolution numerically by using Crank Nicholson implicit finite difference scheme.
4- To determine the effect of van der Waals forces on the stability and rupture of the thin liquid film.

1.5 RESEARCH METHODOLOGY

The linear stability characteristics can be obtained by the solution of the linearized equation of evolution. While linear theory can predict the initial instability however, during the later stages of the growth of instability, nonlinear interactions of antagonistic forces due to gravity, viscosity, thermocapillarity and van der Waals forces assume significance. For the accurate simulations of the nonlinear dynamics and surface morphology of thin-film, we require efficient numerical methods for the solution of the equation of evolution (EOE) (Ali et al., 2005). The extent of nonlinearity and the stiffness of the resulting differential equation depend upon the nature of various physico-chemical effects incorporated in the thin-film. The present work illustrates some results from the numerical simulation of the flow of the thin liquid layer on inclined plane and subjected to evaporative and thermocapillary instabilities. An implicit time averaged Crank Nicholson finite difference formulation of the EOE has been used for numerical simulations. The results from our implicit finite difference code closely match with the Fourier spectral method (Joo et al., 1991) thereby proving the viability of the implicit scheme as a reliable alternative to a spectral method. The validated solution procedure with respect to the published Joo et al. (1991) results has thereafter been employed to study the time evolution of surface instabilities in a non-isothermal thin-film by incorporating the thermocapillarity and evaporation effects besides van der Waals interaction forces.

1.6 SCOPE OF RESEARCH

In this work we aim to investigate the influence of certain physical and chemical effects on the film evolution & stability for the case of a non isothermal thin film flowing on an inclined plane. We utilize certain physical and numerical approximations appropriate for our case to simplify the governing equations in order to arrive at an equation of evolution (EOE) for the film thickness. The analytical and semi-analytical methods of solution of the EOE is beyond our scope, so we resort to numerical solutions. Even then, we will use implicit Crank Nicholson mid-point rule technique, as more advanced numerical techniques such as Fourier spectral or orthogonal collocation are also beyond our scope.

1.7 DISSERTATION ORGANIZATION

Chapter 1 contains an introduction to the background of the problem under study, statement of the problem, research objectives and an outline of the research methodology. Chapter 2 contains the literature review of some aspects of the problem including derivation of governing equations and previous physical and numerical studies. In Chapter 3 the mathematical model is constructed and the governing equations are derived in abridged form. Chapter 4 consists of the numerical solution of the governing equation using implicit Crank Nicholson midpoint method, followed by our conclusions in Chapter 5.

CHAPTER TWO

LITERATURE REVIEW

2.1 THIN FILM MODEL AND GOVERNING EQUATIONS

The linear theory for the isothermal falling film was first studied by Yih (1955) and Benjamin (1957). Yih (1963) was able to calculate the critical Reynolds number above which instability occurs by formulating the problem in terms of long wave asymptotics. Benney (1966) derived a nonlinear equation thus extending the theory into the nonlinear regime. Atherton & Homsy (1976) and Lin & Wang (1985) have discussed a number of extensions of this work. Lin (1974), Sreenivasan & Lin (1978), and Kelly, Davis & Goussis (1986) have incorporated thermocapillarity in the falling film model. Kelly et. al. while considering the linear theory, applied the long wave approximation with arbitrary angle of inclination, and demonstrated that thermocapillarity causes complete destabilization of the film for inclination angles less than 90^o. They also noticed the existence of a stability window; raising or lowering the Reynolds number resulted in destabilization of the stable uniform layer. Joo et al. (1991) have shown that the cause of this phenomenon is the stabilizing effect of hydrostatic pressure, with an analogous phenomenon occurring for evaporative instability as well. For a volatile liquid, another mode of instability can occur due to vapour recoil. Burelbach, Bankoff & Davis (1988) studied this effect recently by considering an evaporating layer with heat transfer, but without gravitational effects. By decoupling the dynamics of the vapour from those of the liquid, they derived an one-sided model of evaporation. Using long-wave theory, they obtained an evolution equation for the static layer, which describes the effects of mass loss (or gain for condensing film), surface tension, van der Waals attractions, vapour recoil, and thermocapillarity. They then focused on the development of dryout, and studied the interaction of the effect of various instabilities on the film rupture.

An active topic of research is the mechanism whereby long wave instabilities occur. These long wave instabilities develop due to the competition between the instability arising due to Marangoni convection when the film is heated below with that of hydrodynamic instability which produces waves when the film flows along an incline. (Joo et al., 1991, 1996; Kabov et al., 1995, 1999, 2001, 2002; Kalitzova-Kurtova et al., 2000; Slavtchev et al., 2001; Miladinova et al., 2002; Kalliadasis et al., 2003a, 2003b; Trevelyan and Kalliadasis, 2004; Scheid 2004). The instability that occurs due to the interaction and competition between thermocapillarity and long wave hydrodynamic instabilities in a film that is flowing across a uniformly heated planar surface has been investigated by Goussis and Kelly (1991). They discovered that the film is influenced not only by the hydrodynamic mode of instability but also by the thermocapillarity instability modes. Also, experimental investigations of falling thin liquid films on heated planar surfaces show the occurrence of new instabilities not seen before (Kabov et al., 1995, 2003). Joo et al., (1991) have studied a two dimensional theory of uniform thin film layers of a volatile liquid film flowing down a uniformly heated inclined plane by using a Benney type equation of evolution for the local film thickness. Their time dependent computations showed wave breaking due to the effects of evaporative instability, surface wave instability and thermocapillarity instability which led to the rupture of the film.

2.2 NUMERICAL SOLUTION

Numerous works on numerical simulations of various liquid thin-film models have been reported in the literature [e.g., 12, 13, 14, 15]. Burelbach et al. (1988) has solved the problem of evaporating/condensing liquid film on horizontal plane using an implicit finite difference scheme, Crank-Nicholson mid-point rule, by employing centered difference for space and forward difference for time derivatives. The resultant nonlinear difference equations are solved by Newton-Raphson iterations. Ali et al. (2005) have employed similar discretization scheme for their isothermal liquid thin-film on inclined plane, however IMSL subroutines were employed for the solution of resulting difference equations which essentially uses an adoption of Newton-Raphson method. Fourier spectral method was used by Joo et al. (1991) for numerical simulations of heated falling films under the influence of thermocapillarity and evaporative effects at the surface, however, they have ignored van der Waals effects in their formulation. Jameel (1994) used Fourier collocation method for the simulation of thin fluid films on horizontal substrates under the influence of antagonistic apolar and polar forces. A long wave analysis of the equations of mass, energy and motion by has been performed by Peramanu and Sharma (1998) to investigate the nonlinear stability and dynamics of nonisothermal falling films with simultaneous absorption from a gas phase. The resulting evolution equation for the film thickness had been solved by a Fourier collocation technique and the nonlinear stability and dynamics were characterized. Zope et al. (2001) and Bandyopadhyay and Sharma (2007) employed finite difference scheme to discretize the space derivatives using central differencing with half node interpolation. The resultant sets of ordinary differential equations in time were integrated using Gears algorithm. An explicit finite difference scheme using centred staggered differencing for space derivatives was employed by Ramos-de-Souza (2001) for the thin film bounded by a viscous phase with charged surfactants. Later in 2007, Fisher and Golovin carried out numerical simulations of their two-layer thin film with surfactants model using an explicit finite difference conservative scheme. They employed first order in time and second order in space finite difference using 40 grid points per one wavelength with a time step of 10^{-4}. In 2005, Miladinova and Lebon (2005) studied dynamics of two-dimensional evaporating film on an inclined plate by numerical simulations. They used Crank-Nicholson mid-point rule in time, and upwind difference for convective terms while second and fourth order derivatives were discretized using centered differences.

These are certainly not an exhaustive coverage of all such works reported in the literature. There are many other works that have been reported in the literature. Oron, Gottlieb and Novbari (2009) studied the nonlinear dynamics of thin liquid films falling on a vertical oscillating plane numerically using a weighted residual integral boundary layer model. Stability of viscoelastic thin liquid films was studied using momentum integral method by Dandapat et al. (2003), Mukhyopadhyay et al. (2008) and Uma and Usha (2006). Sirwah and Zakariah (2013) studied the hydrodynamic instability of a thin condensate viscoelastic liquid film flowing down on the outer surface of an axially moving vertical cylinder. In Sadiq et al. (2010), the stability of a thin viscous Newtonian fluid draining down a uniformly heated porous inclined plane was investigated. Solimah and Alhumaizi (2013) studied the dynamics of coating thin films on horizontal stationary and rotating cylinders in general and when the effect of van der Waals forces is significant. In this case the authors found that the positive van der Waals forces caused rupture of the film with the rupture time of the film decreasing with increase of van der Waals forces. On the other hand gravity has a stabilizing effect and increases rupture time.

2.3 APPLICATIONS

In biophysics, thin films are present as membranes, as linings of mammalian lungs (Grotberg, 1994), or as tear films in the eye (Sharma and Ruckenstein, 1986a; Wong *et al.*, 1996). They occur in Langmuir films (Gaines, 1966) and in foam dynamics (Bikerman, 1973; Edwards *et al.*, 1991; Schramm and Wassmuth, 1994; Wasan *et al.*, 1994; Wong *et al.*, 1995). In engineering, thin films contribute to limit fluxes and protect surfaces in heat and mass transfer processes, and their applications arise in paints, adhesives, and membranes. Thin films are used as lubricating layers for the flow of crude oil in channels and pipes. They are also commonly used for cooling of microelectronic equipment.

2.4 SUMMARY

According to our literature review, even though finite difference methods have been reported in previous studies of the problem, it seems that implicit finite difference methods have not yet been applied to the problem at hand. Moreover, the effect of van der Waals forces on film evolution and thickness has been neglected as of yet. We wish to demonstrate the reliability of implicit numerical methods for such kinds of problems and also to study the influence of van der Waals forces in such problems.