A Comparative Study of Two Different Numerical Schemes for the Simulation of Nonlinear Dynamics of Heated Falling Thin Films

Mohammad A. Hamza, Ahmad T. Jameel, Waqar Asrar

Abstract— In this research, an attempt is made to characterise qualitatively the stability and dynamics of an inclined thin liquid film under the influence of instabilities due to thermo-capillarity and evaporative effects as well as van der Waals intermolecular forces, by employing the implicit finite difference method. The results are compared with solutions obtained by the Fourier spectral method. Flow in thin films of a Newtonian liquid on an inclined plane with an adjacent passive gas layer, is well represented by the Navier-Stokes equations, equation of continuity and associated boundary conditions. Long-wave (lubrication) approximation is applied to simplify the governing equations to arrive at a nonlinear partial differential equation, called equation of evolution (EOE). The spatio-temporal evolution of the interfacial instability in the film caused by internal and/or external effects are studied by numerically solving the EOE using the implicit finite difference method. The results of the numerical simulations of our thin film model are compared with those of a similar problem solved using Fourier spectral method from the literature. Simulations show remarkable agreement in the film dynamics predicted by these two methods. The film rupture times obtained using our implicit finite difference scheme closely match with the values obtained from the Fourier spectral method within less than 1% error. This implies that the implicit finite difference method can be satisfactorily employed for the efficient numerical simulation of the thin film flows, and to decipher its nonlinear dynamics reliably.

Keywords: Implicit finite difference; Long-wave instability; Nonlinear dynamics; Spectral method; Thin liquid film.

1. INTRODUCTION

Thin liquid films find wide applications in science and engineering. A liquid film may be considered thin if its thickness is much smaller than its lateral dimensions. In engineering, thin films occur in heat and mass transfer processes and serve to limit fluxes and to protect surfaces, and finds applications in adhesives, paints, tear films and biological 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 also develop wave motion. The interfacial waves in a thin film 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 solid surface to the atmosphere. Thin film flows are governed to a good approximation by the equations of motion simplified by the long wave (lubrication) approximation.

The stability and nonlinear dynamics of flow of thin liquid films on solid planes has been studied extensively over the past decades. Especially, thin liquid films subjected to various physical-chemical effects such as instabilities due to evaporation at the surface, thermocapillarity, and solutal Marangoni effects owing to thermal gradient in the film had been focus of some of the past and recent works. Furthermore, for an inclined film, the effect of gravitational force becomes significant enough to influence the nonlinear dynamics of the film coupled with other forces. There are numerous applications of inclined thin films in industries, such as thin film heat exchangers, falling film gas-liquid contact devices, sodium cooled fast reactors and many more. Especially, heat transfer in inclined thin liquid film flow is of importance in various chemical and biochemical processes such as solid coating, food processing and in systems with evaporative cooling/condensation as well as high throughput heat 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 [1-6].
In what follows, we present the results of our numerical simulations of flow in thin liquid films under the influence of intermolecular van der Waals force, thermo-capillary effect and evaporative instabilities at the free surface. Flow in thin Newtonian liquid film on a solid plane and confined by an adjacent passive gas layer is represented by equation of motion, equation of continuity and associated boundary conditions. The external effects due to gravity and van der Waals attraction are generally incorporated in the body force term of the Navier-Stokes equation. These governing equations rewritten using new variables as defined in Hamza [11], are first rescaled using lubrication theory and then simplified using the long-wave analysis of Benny [7] to arrive at a nonlinear partial differential equation, henceforth called the equation of evolution (EOE) [3, 7-11]. The time evolution of the interfacial instability of the film caused by internal and/or external effects was obtained by numerically solving the EOE [10, 11].

To delineate the detailed nonlinear dynamics and surface morphology of thin-film subjected to different type of instabilities, one requires a robust and efficient numerical scheme for the solution of the equation of evolution (EOE). An implicit time-averaged finite difference formulation of the EOE using Crank Nicholson scheme has been used for the numerical solution of our thin-film model. It is interesting to note that the simulation results obtained using our implicit finite difference code greatly conform with the Fourier spectral simulations of Joo et al. [8], as shown in the results section. This clearly proves the efficacy of the implicit finite difference scheme as a reliable alternative to the Fourier spectral method. The results of the finite difference code used in the present work, was validated with respect to the published results of Joo et al. [8] that employed Fourier spectral method. Thereafter, numerical simulations were carried out using our computer code to study the time evolution of surface instabilities in a non-isothermal thin-film by incorporating the gravity and van der Waals forces, besides thermo-capillary and evaporative effects on the surface [10, 11].

2. METHODS

The brief description of the physics of the problem and its mathematical formulation are given in the following paragraphs.

2.1 The thin film model

Consider a thin viscous Newtonian liquid film resting on a uniformly heated rigid plate inclined at angle θ to the horizontal and bounded above by its vapour as shown in Fig. 1. Film is thick enough that a continuum theory of the liquid is applicable. The film is laterally unbounded and has constant material properties. The mean film thickness is $h_0$. The layer is evaporating so that at the vapour-liquid interface there is mass loss, momentum transfer and energy consumption. The plate has a fixed constant temperature TH. Evaporative losses to the passive gas above controls the liquid temperature, TF on the free surface. The surface tension, $\sigma_0$ is a function of temperature, so that the thermo-capillary effects are present. The flow in the thin film can be represented by the Navier-Stokes, energy and continuity equations using a two-dimensional Cartesian co-ordinate system $(x, z)$, together with no-slip condition at the solid surface, and the normal and shear stress conditions at the free surface, and the constitutive equation.

Following the analysis in Burelbach et al. [9] and Joo et al. [8], the governing equations for motion in thin film can be simplified under long wave approximation, to arrive at a nonlinear fourth order partial differential equation, called the ‘equation of evolution’ [EOE] that describes the evolution of the film interface in time t, and space x, denoted by $h(x,t)$, and is given by [8-12].

$$
\frac{h_t}{h + \epsilon} + Gh^2 h_x \sin \theta + \left[ \frac{2}{15} G h^6 h_x \sin^2 \theta + \frac{K \mu}{(h+k)^2} + \frac{E^2}{D(h+k)^2} - \frac{1}{3} G h^3 h_x \cos \theta + \frac{A}{h} h_x + Sh^3 h_{xxx} \right] + \frac{5}{24} GE \left( \frac{h^4}{h+k} \right)_x \sin \theta + \frac{EP}{3(h+k)} \left[ \frac{E}{3(h+k)} + \frac{G}{120} (7h - 15K) h h_x \sin \theta \right] = 0
$$

(1)

The definitions of symbols used in Eq. 1 are given in Appendix 1. The subscripts, t and x represent the derivatives with respect to time, t and space coordinate x respectively. Eq. 1 can be solved for the film thickness $h(x, t)$ using a space periodic initial condition,

$$
h(0, x) = 1 - \epsilon \cos kx ; \quad |\epsilon| < 1
$$

(2)

with periodic boundary conditions in x-domain over a disturbance wavelength, $\lambda = 2\pi/k$, where k is a wavenumber, and $\epsilon$ is the amplitude of the initial perturbation on the film surface. For a cosine wave initial condition, the boundary conditions can be expressed as [8-12].

$$
\left( \frac{\partial^n h}{\partial x^n} \right)_{x=-\lambda/2} = \left( \frac{\partial^n h}{\partial x^n} \right)_{x=\lambda/2} (i = 0, 1, 2, 3);
$$

$$
-\lambda/2 \leq x \leq \lambda/2
$$

(3)
2.2 Equation of evolution by Joo et al. [8]

The EOE of Joo et al. [8] is rewritten here for ease of reference and clarity of results presented later in the paper. The EOE is:

\[
\frac{\partial h_i}{\partial t} + \frac{h_i}{h_{i+1} + K} + G h_i^2 \sin \theta + \varepsilon \left( \frac{\varepsilon^2 h_i^2 \sin^2 \theta}{2} + \frac{K M h_i^2}{p (h_{i+K})^2} + \frac{E^2 h_i^2}{D (h_{i+K})^3} - \frac{1}{3} G h_i^3 \cos \theta + Sh_i^3 \right) + \frac{5G}{24} \left( \frac{h_i}{h_{i+K}} \right) \sin \theta + e \frac{\varepsilon E}{(h_{i+K})^3} \left[ \frac{\varepsilon}{(3h_{i+K})^2} + \frac{a_5}{120} (7h_i - 15K) h_i \sin \theta \right] = 0
\]

Equation (4) can be scaled back to the original non-dimensional coordinates (x, z, t) and unscaled parameters E, D, and S using following scale factor used by Joo et al. [8], and becomes identical with our EOE (Eq. 1) except that the term owing to van der Waals effect is absent in Joo et al. [8].

The implicit finite difference scheme are compared with those of Fourier spectral method of Joo et al. [8].) The implicit finite difference scheme employed by Joo et al. [8] is rewritten here for ease of reference and clarity of results presented later in the paper.

2.2.1 Equation of evolution by Joo et al. [8] rewritten

The EOE of Joo et al. [8] is rewritten here for ease of reference and clarity of results presented later in the paper. The EOE is:

\[
\frac{\partial h_i}{\partial t} + \frac{h_i}{h_{i+1} + K} + G h_i^2 \sin \theta + \varepsilon \left( \frac{\varepsilon^2 h_i^2 \sin^2 \theta}{2} + \frac{K M h_i^2}{p (h_{i+K})^2} + \frac{E^2 h_i^2}{D (h_{i+K})^3} - \frac{1}{3} G h_i^3 \cos \theta + Sh_i^3 \right) + \frac{5G}{24} \left( \frac{h_i}{h_{i+K}} \right) \sin \theta + e \frac{\varepsilon E}{(h_{i+K})^3} \left[ \frac{\varepsilon}{(3h_{i+K})^2} + \frac{a_5}{120} (7h_i - 15K) h_i \sin \theta \right] = 0
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Equation (4) can be scaled back to the original non-dimensional coordinates (x, z, t) and unscaled parameters E, D, and S using following scale factor used by Joo et al. [8], and becomes identical with our EOE (Eq. 1) except that the term owing to van der Waals effect is absent in Joo et al. [8].

2.3 Numerical formulation

To fully characterize the nonlinear dynamic behaviour of flow in the heated thin film on an inclined plate, one needs to solve numerically the evolution equation (Eq. 1) for a wide range of parameter values representing different thermo-physical states. Thus we need a robust numerical method to solve Eq. 1 reliably and efficiently. Hamza et al. [10] and Hamza [11] have used implicit Crank Nicholson method to solve Eq. 1 reliably and efficiently. Hamza et al. [10,11,13] using our implicit code are compared with those of Fourier spectral method employed by Joo et al. [8].) The implicit finite difference scheme - Crank-Nicholson mid-point rule is briefly described in the following paragraph.

2.3.1 Implicit finite difference scheme - Crank-Nicholson Mid-Point Rule

The rescaled equation of evolution (Eq. 1) is discretized in its conservative form using forward difference in time and central difference in space with time averaging, resulting into a set of difference equations for the film thickness h(x,t) in [10,11,13]. These equations are then solved as a set of nonlinear coupled algebraic equations by an iterative procedure of the type of Newton’s method. Let subscript i denotes the space discretization and superscripts n and n+1 denote values of variables at nth and (n+1)th times. Thus, Eq. 1 after discretization and simplification appears as:

\[
\begin{align*}
\frac{h_{i+1} - h_i}{\Delta t} + a_1 \frac{h_{i+1} - h_i}{h_{i+1} + K} + a_2 h_i^2 \left( h_{i+1} - h_{i-1} \right) + a_3 \left( h_{i+1}^3 - h_i^3 \right) - h_{i+1}^2 \left( h_{i+1} - h_{i-2} \right) + a_4 \left( h_{i+1}^2 - h_i^2 \right) & = a_5 \left( h_{i+1}^2 h_{i+2} - h_i^2 \right) + a_6 \left( h_{i+1}^2 - h_i^2 \right) + a_7 \left( h_{i+1}^2 - h_i^2 \right) + a_8 \left( h_{i+1}^2 - h_i^2 \right) \\
\end{align*}
\]

The constants a_i (i=1,2, 3, ......., 12) are defined as:

\[
\begin{align*}
a_1 &= \frac{SE}{2A^2}, \quad a_2 = \left( \frac{S}{A} \right)^2 \frac{Re}{4DA}, \quad a_3 = \frac{\Delta t}{4(Ax)^2} 15A', \\
a_4 &= \frac{GM}{8(\Delta x)^2} PA', \quad a_5 = \frac{GM}{8(\Delta x)^2} DA', \\
a_6 &= \frac{GM}{8(\Delta x)^2}, \quad a_7 = \frac{GM}{8(\Delta x)^2}, \quad a_8 = \frac{GM}{8(\Delta x)^2}, \\
a_9 &= \frac{\Delta t}{4Ax} \left( \frac{S}{A} \right)^2, \quad a_{10} = \frac{\Delta t}{2(\Delta x)^2} EP, \\
a_{11} &= \left( \frac{S}{A} \right)^2 \frac{E}{3}, \quad a_{12} = \frac{Re}{240Ax} \\
\end{align*}
\]

Eq. (5) forms a set of coupled nonlinear algebraic equations which were solved iteratively using Newton Raphson method on the MATLAB platform [14]. Twenty-one grid points in spatial domain and a time step of 0.001 was used throughout the simulations as it was found sufficient for a converged solution for the parameters investigated as evident from the mesh sensitivity analysis given in the next section. The values of physical parameters used in simulations are given in Appendix 2.

3. RESULTS AND DISCUSSION

The results of the numerical solution of the equation of evolution (EOE) given in Eq. 1 (with the van der Waals force term deleted, reduces our EOE identical to that of Joo et al. [7]) using our implicit code are compared with the numerical results from Fourier spectral method of Joo et al. [7], in figures 2 through 5. Fig. 2 depicts the gravitational instability for an isothermal layer (E = E2/D = KM/P =0) for a wave number k=0.7.
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The free surface profiles for the time, $\tau = 0 - 2$ are almost identical to that of Joo et al. [7]. Each profile represents a time increment of 0.05, with the final profile (shown in red colour) corresponds to $\tau = 2$.

Evolution of the free surface profiles for the layer with thermo-capillarity for $k=0.7$ and corresponding to $G=5$, $\beta=30^0$, $KM/P=1$, $K=0.1$, $\bar{S}=0.1$, $\bar{E} = E^2/D = KM/P = 0$ are shown in Fig. 3 for the time range $0 \leq \tau \leq 2.9$, with a time increment of $\Delta \tau = 0.1$. It may be noted that the film interface profiles are remarkably similar for the simulations based on FDM (present work) and the Spectral method (Joo et al. [7]). The profile shown in red corresponds to the last time step in each case.

Fig. 4 shows the evolution of the film interface for an evaporating layer where various nonlinear antagonistic forces lead to instability resulting into the film rupture. The interface profiles are shown for $\Delta \tau = 0.05$, and for parameter values shown in the figure caption. Our film rupture time, $\tau_R$ obtained using implicit FDM is 4.9384 that exactly conform to the rupture time $\tau_R = 4.9388$ from spectral method (Joo et al. [7]) with numerical accuracy up to 3rd decimal place.

Figures 5 shows the free surface profiles for evaporating layers with gravitational effects leading to rupture for an inclination, $\theta = 15^0$. Parameters are: $k=0.7$, $\bar{E}=0.1$, $K=0.1$, $P=1$, $\bar{S}=0.1$, $G=5$, $E^2/D=0.0005$, $KM/P=1$, $M=1$, with $\Delta \tau = 0.05$. Rupture time $\tau_R$ from FD simulations is 5.1290. The rupture time $\tau_R$ from the spectral method (Joo et al. [7]) is 5.1525. The maximum deviation between values of rupture times obtained from FD method (present work) and spectral method (Joo et al. [7]) was observed to be 0.46%.
4.1 Mesh sensitivity analysis

The mesh sensitivity analysis for our implicit scheme was performed for the liquid layer in Fig. 4. The simulations were carried out until dry out using parameters of Fig. 4 ($k = 0.7, G=0, KM/P=0, E=0.1, K=0.1, P=1$, and $S=0.1$), for decreasing time steps, i.e., $\Delta \tau = 0.01, 0.05, 0.001, 0.005$ and $0.0001$, and increasing number of grid points, i.e., $N=21, 31, 41$ and $51$ as shown in Table 1. It is evident from the rupture time shown in the table that the numerical solution converges (up to third decimal place) at $N = 21$ and $\Delta \tau = 0.001$ for the film investigated.

<table>
<thead>
<tr>
<th>$\Delta \tau$ (time step)</th>
<th>$N$ (grid points)</th>
</tr>
</thead>
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<tr>
<td></td>
<td>21</td>
</tr>
<tr>
<td></td>
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<tr>
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<td>0.005</td>
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<td>0.0001</td>
<td>29.49347</td>
</tr>
</tbody>
</table>

CONCLUSIONS

We have shown comparison between an implicit finite difference scheme and Fourier spectral method applied to the problem of a thin liquid film flowing down an inclined plane subject to various physicochemical effects. These include gravity, thermo-capillarity, evaporative instabilities, surface tension and van der Waals forces. In order to solve the
nonlinear evolution equation describing the dynamics, we have employed the implicit Crank Nicholson midpoint scheme and compared the results to those of Joo et al. [8] that employed Fourier spectral method. In the case where the effect of van der Waals forces are neglected, our results seem to reproduce closely the results of Joo et al. [8], with only occasional slight deviation. The cases where the instabilities lead to film rupture, the rupture time obtained using implicit FD method are in close agreement with those obtained by Joo et al. [8] within a deviation less than 1%. The cases where rupture is not reported, the film surface profiles at various times of deformation are almost identically similar in the two cases, i.e., implicit FD and spectral methods. Further, the mesh sensitivity analysis show that the numerical solutions converged for the time step 0.001 and 21 spatial grids. This implies that implicit finite difference method using Crank-Nicholson mid-point rule represents a reliable alternative method for the study of nonlinear dynamics and stability of non-isothermal thin film on inclined plane.

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REFERENCES


Appendix 1

Non-dimensional Parameters Occurring in the Mathematical Model

Non dimensional mean surface tension, \( s = \frac{\sigma_{\mu}}{3\rho v^2} \)

Evaporation number, \( E = \frac{\kappa\Delta T}{\rho L} \)

Non dimensional Hamaker constant, \( A = \frac{A'}{6\sigma_{\mu}\rho v^2} \)

Non dimensional gravitational number, \( G = \frac{h\rho g}{\sigma_{\mu}} \)

Thermal diffusivity, \( \kappa = \frac{k_t}{\rho c_p} \)

Marangoni number, \( M = \frac{\gamma_{\mu}}{2\mu K} \)

Prandtl number, \( P = \frac{\alpha}{k_t} \)

Ratio of vapour to liquid density, \( D = 10^{-3} \)

Reynolds number, \( Re = G \sin \theta \)

Appendix 2

Nomenclature and Numerical Values of Various Parameters Used in Simulations

\( \Delta t \) (time step in simulation) = 0.001

\( \rho \) (liquid density) = 1000 kg/m³

\( k_t \) (liquid thermal conductivity) = 0.613 W/m.K

\( K \) (a parameter that measures the degree of non-equilibrium at the evaporating interface) = 0.1

\( c_p \) (liquid thermal conductivity) = 4.19 kJ/kg.K

\( L \) (latent heat of vaporization) = 2257 \times 10^3 / kg

\( \nu \) (liquid kinematic viscosity) = 0.3548 \times 10^{-6} m²/s

\( \mu_\mu \) (liquid viscosity) = 0.3548 \times 10^{-3} kg/m.s

\( \Delta T \) (\( T_1 - T_2 \)) = 20K

\( \gamma \) (\( \frac{\partial s}{\partial t} \)) = 0.18 \times 10^{-3} N/m.°C

\( \Delta A \) (Hamaker constant, dimensional) = 4.67 \times 10^{-20}J

\( \sigma_{\mu} \) (mean surface tension at the saturation temperature) = 72.8 \times 10^{-3} J/m²

\( \varepsilon \) (amplitude of initial disturbance on the film surface) = 0.1