Simulation of Flow Regimes of Non-isothermal Liquid Films

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Abstract. For moderate Reynolds numbers, a nonlinear partial differential equation of the free surface state of a non-isothermal liquid film is presented. The algorithm was developed and the program was written in Matlab R2017b using the Symbolic Math Toolbox module. The wave characteristics of the liquid film under heat and mass transfer are calculated. The flow regimes of a vertical liquid film with a maximum perturbation growth rate are distinguished, and the effect of temperature gradients and surface viscosity on them is investigated.

Keywords: Liquid film · Non-linear mathematical model · Instability · Increment

1 Introduction

Studies of thin viscous liquid layers (liquid film) flows are carried out both theoretically [1–3,9,11,12,18,21] and experimentally [2,4–8,10]. The relevance and practical significance of these studies are associated with the implementation of liquid film flows in numerous devices, for example, in evaporators, absorbers, distillation columns, crystallizers, refrigeration equipment, as well as liquid film is the basis of many technological processes in chemical, petrochemical, food and other industries [14,15]. Low thermal resistance and a large contact surface at low specific fluid flow rates make liquid film a very effective tool in the process of interfacial heat and mass transfer. In addition, in many cases there is an additional intensification of transport processes due to wave formation. Various physical and chemical factors, such as temperature effects (temperature gradients) and the presence of insoluble surfactants (surface viscosity) on the free surface of the film affect the wave characteristics of the liquid film and the process of wave formation [5,13,14,19,20,22]. Experimental studies of the flow regimes of liquid films [14,16] show that the regimes with the maximum value of the increment are the most stable with respect to small perturbations. The maximum value of the increment and the corresponding wave number determine the optimal flow regime of the liquid film. Mathematical modeling of optimal flow regimes of liquid films allows us to determine the influence of various physical and chemical factors on the corresponding wave characteristics.

The novelty of the study is related to the effect of temperature gradients and surface viscosity on the wave characteristics of the liquid film.

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2 Mathematical Model

We consider the flow of a thin viscous liquid layer with a free surface under the action of gravity on a solid impermeable surface with a temperature T in the coordinate system OXY (Fig. 1), where the OX axis is directed in the direction of the layer flow and the OY is directed perpendicular to the liquid layer. Presence of insoluble surfactants on the free surface of the liquid film was also taken into account. Liquid film is described by the system of Navier-Stokes equations and the continuity equation with boundary conditions [20,22].

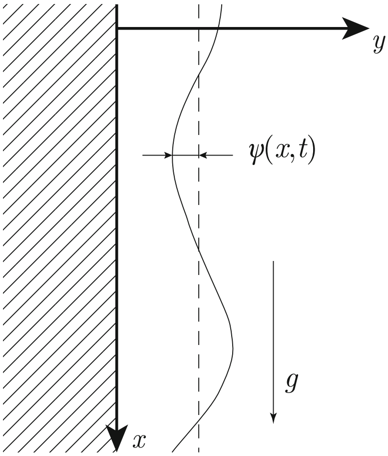

Fig. 1. Flow of liquid film.

The nonlinear mathematical model of the state of the free surface of the liquid film for moderate Reynolds numbers has the form [20]:

$$\begin{aligned}
&\left(a_7\frac{\partial}{\partial x}+a_{13}\right)\frac{\partial\psi}{\partial t}+a_1\frac{\partial^4\psi}{\partial x^4}+a_4\frac{\partial^3\psi}{\partial x^3}+a_6\frac{\partial^2\psi}{\partial x^2}+a_{11}\frac{\partial\psi}{\partial x}\\
&+a_{14}\psi\frac{\partial\psi}{\partial x}+a_{16}\psi\frac{\partial^2\psi}{\partial x^2}+a_{17}\psi\frac{\partial^2\psi}{\partial x\partial t}+a_{21}\frac{\partial\psi}{\partial x}\frac{\partial\psi}{\partial t}+a_{22}\left(\frac{\partial\psi}{\partial x}\right)^2\\
&+a_{26}\frac{\partial\psi}{\partial x}\frac{\partial^2\psi}{\partial x^2}+a_{28}\psi\frac{\partial^3\psi}{\partial x^3}+a_{30}\frac{\partial\psi}{\partial x}\frac{\partial^3\psi}{\partial x^3}+a_{34}\psi\frac{\partial^4\psi}{\partial x^4}+a_{37}\psi^2\frac{\partial\psi}{\partial x}\\
&+a_{39}\psi^2\frac{\partial^2\psi}{\partial x^2}+a_{40}\psi^2\frac{\partial^2\psi}{\partial x\partial t}+a_{44}\psi\frac{\partial\psi}{\partial x}\frac{\partial\psi}{\partial t}+a_{45}\psi\left(\frac{\partial\psi}{\partial x}\right)^2\\
&+a_{49}\frac{\partial\psi}{\partial x}\frac{\partial^2\psi}{\partial x^2}+a_{51}\psi\frac{\partial\psi}{\partial x}\frac{\partial^3\psi}{\partial x^3}+a_{55}\psi^2\frac{\partial^4\psi}{\partial x^4}+a_{58}\psi^2\frac{\partial^3\psi}{\partial x^3}=0
\end{aligned}\tag{1}$$

The coefficients of Eq. (1) include physical and chemical parameters: Re—Reynolds number, F_x—Froude number, σ—surface tension, M—temperature gradients, N—surface viscosity.

$$\begin{aligned}
&a_1 = -\frac{Re\sigma}{3}, a_4 = -\frac{Re^2 F_x N}{2},\\
&a_6 = -\frac{ReF_y}{3} - \frac{ReM}{2} + \frac{3}{40}Re^3F_x^2, a_7 = \frac{5}{24}Re^2F_x,\\
&a_{11} = -ReF_x, a_{13} = -1, a_{14} = -2ReF_x,\\
&a_{16} = -ReF_y - ReM + \frac{9}{20}Re^3F_x^2, a_{17} = \frac{5}{6}Re^2F_x,\\
&a_{21} = a_{17}, a_{22} = a_{16}, a_{26} = -\frac{1}{2}Re^2F_xN, a_{28} = 3a_{26},\\
&a_{30} = a_{34} = -Re\sigma, a_{37} = -ReF_x,\\
&a_{39} = -ReF_y - \frac{ReM}{2} + \frac{9}{8}Re^3F_x^2,\\
&a_{40} = \frac{5}{4}Re^2F_x, a_{44} = 2a_{40}, a_{45} = -2ReF_y, a_{49} = -Re^2F_xN,\\
&a_{51} = -2Re\sigma, a_{55} = \frac{1}{2}a_{54}, a_{58} = -\frac{3}{2}Re^2F_xN.
\end{aligned} \tag{2}$$

We consider the linear part of Eq. (1). Using the solution type $\psi(x,t) = A\ exp\ i(k_x x - \omega t)$, we obtain the dispersion equation

$$\omega(a_7k_x + i) + a_1k_x^4 - a_4ik_x^3 - a_6k_x^2 + a_{11}ik_x = 0. \tag{3}$$

Let us split real and imaginary parts of Eq. (3) and get the solutions for increment ω_i and phase velocity c_r

$$\omega_r = \frac{Y - XZ}{1 + Z^2}, \tag{4}$$

$$\omega_i = X + \omega_r Z, \tag{5}$$

$$c_r = \frac{\omega_r}{k_x}, \tag{6}$$

where $X = a_1k_x^4 - a_6k_x^2$, $Y = a_4k_x^3 - a_{11}k_x$, $Z = a_7k_x$.

Numerical study of liquid film flows for the range of Reynolds numbers [1,15] in the framework of Eq. (3) allows to solve a number of important problems:

1. Finding areas of instability of the flow of non-isothermal liquid films under the influence of various physical and chemical factors, such as temperature gradients and surface viscosity.

2. Selection of optimal flow regimes of liquid films. Optimal modes are flow regimes of liquid film with a maximum value of the increment. Optimal flow regimes are needed for correct operation of heat and mass transfer devices.
3. Calculation of phase velocity and wavelength for wave numbers corresponding to optimal flow regimes.

We present a model of the algorithm for calculating the wave characteristics.

for $Re = 5$ **to** 15 **do**
  Compute equation coefficients $a_1, a_2, ..., a_{58}$
  Construct symbolic expressions for ω_i, c_r
  Get first derivatives for ω_i, c_r
  Compute roots of derivatives
  print $k_{x_{max}}, \omega_{i_{max}}, c_{r_{min}}$
end for

3 Computational Experiments

Unstable modes of liquid films are characterized by positive values of increment. On the increment curve (Fig. 2), the following points could be noted: the maximum value of the increment and the zero value of the increment with the corresponding wave numbers. The set of points k_{max} for the studied range of Reynolds numbers form the curve of the maximum growth of disturbances (Fig. 3) and the set of points k_0—neutral stability curve.

For the free flow of a liquid film of water, Table 1 presents maximum values of the increment, wave number and wavelength.

Phase velocity of the liquid film in the region of instability varies within the limits $2 \leq c_r \leq 3$, which corresponds to the experimental data of the authors [4–7]. Figure 4 shows values of minimal phase velocity that correspond to the regime with the maximum value of increment.

Table 1. Optimal regimes of the flow

Re	$\omega_{i_{max}}$	k_{max}	λ
5	0.015357	0.072459	86.713455
6	0.023877	0.083407	75.331313
7	0.033763	0.093321	67.328672
8	0.044279	0.102114	61.531077
9	0.054640	0.109758	57.245706
10	0.064189	0.116292	54.029236
11	0.072502	0.121807	51.583077
12	0.079388	0.126422	49.700115
13	0.084838	0.130264	48.234194
14	0.088956	0.133455	47.080929
15	0.091903	0.136103	46.164965

Table 2. Optimal flow regimes of film falling over the heated surface

Re	$\omega_{i_{max}}$	k_{max}	λ
5	0.030210	0.085813	73.219488
6	0.046217	0.098381	63.865784
7	0.063997	0.109499	57.381366
8	0.081920	0.119092	52.759059
9	0.098542	0.127194	49.398544
10	0.112905	0.133926	46.915380
11	0.124586	0.139461	45.053350
12	0.133577	0.143985	43.637913
13	0.140113	0.147671	42.548412
14	0.144543	0.150675	41.700353
15	0.147236	0.153122	41.033778

Table 3. Optimal flow regimes of film with insoluble surfactants

Re	$\omega_{i_{max}}$	k_{max}	λ
5	0.029069	0.084120	74.693091
6	0.043593	0.095363	65.887001
7	0.059045	0.104714	60.003557
8	0.073901	0.112144	56.027958
9	0.086995	0.117757	53.357396
10	0.097706	0.121748	51.608198
11	0.105892	0.124356	50.525784
12	0.111732	0.125823	49.936514
13	0.115556	0.126373	49.719269
14	0.117740	0.126199	49.787755
15	0.118636	0.125465	50.079185

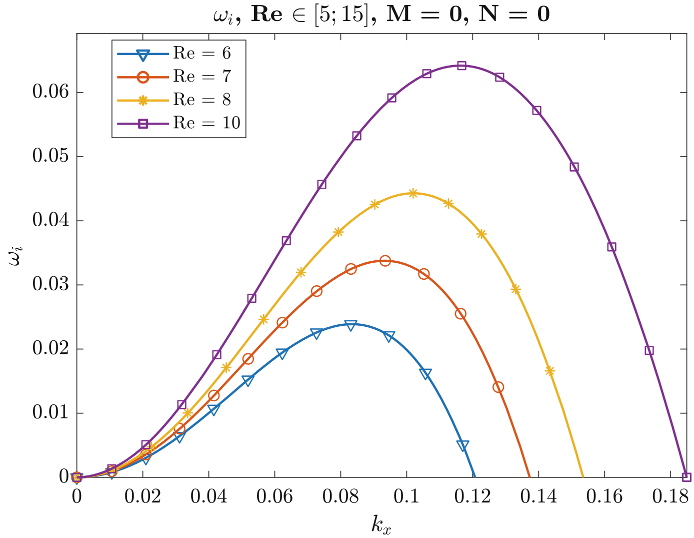

Fig. 2. Increment of liquid film.

We investigate the effect of temperature gradients arising during the flow of the liquid film over the heated surface. This flow is characterized by increase in values of the increment (Fig. 5) and a decrease in the values of phase velocity (Fig. 6). Table 2 shows wave characteristics of optimal film flow regimes. In region of instability of the liquid film, depending on the magnitude of the temperature gradients, rupture of film is possible. In Fig. 7 critical values of the temperature gradients are presented, where possible gaps in film structure could lead to emergency modes [17].

The presence of insoluble surfactants (oils, fats) on the free surface of film leads to stabilization of the flow. The increment value is significantly reduced (Fig. 8), while phase velocity increased (Fig. 9). Table 3 shows wave characteristics of optimal water film flow with insoluble surfactants present.

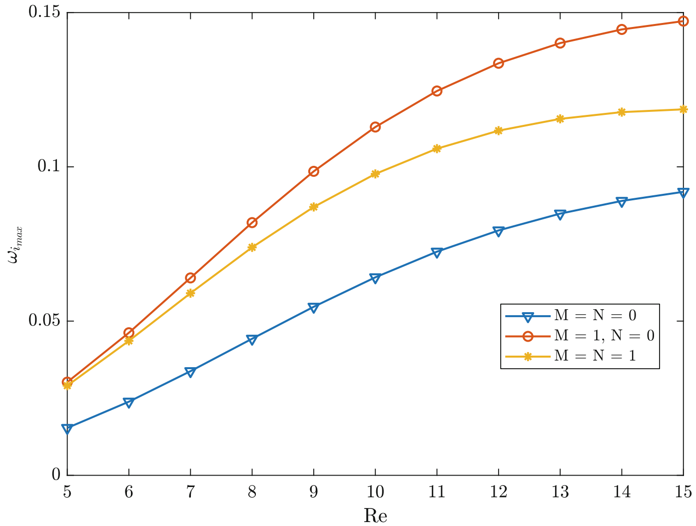

Fig. 3. Curve of the maximum growth of disturbances.

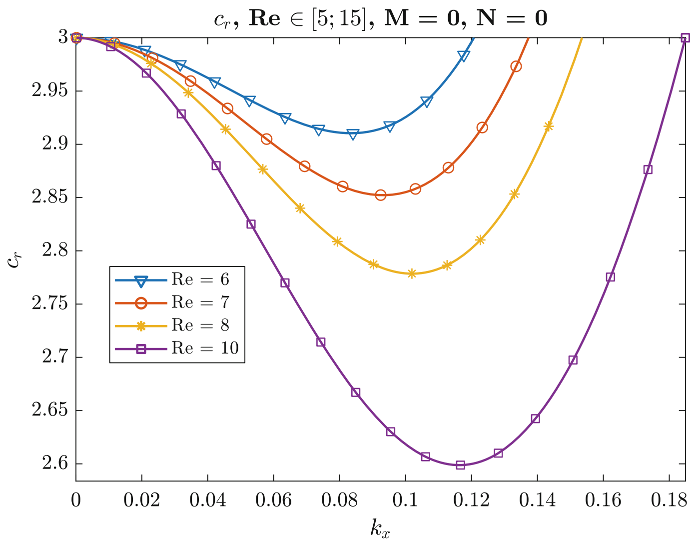

Fig. 4. Phase velocity of liquid film.

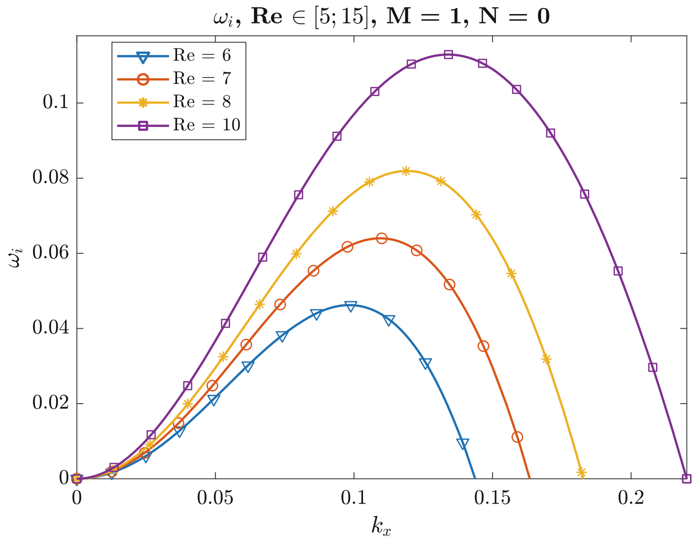

Fig. 5. Increment of liquid film flowing over the heated surface.

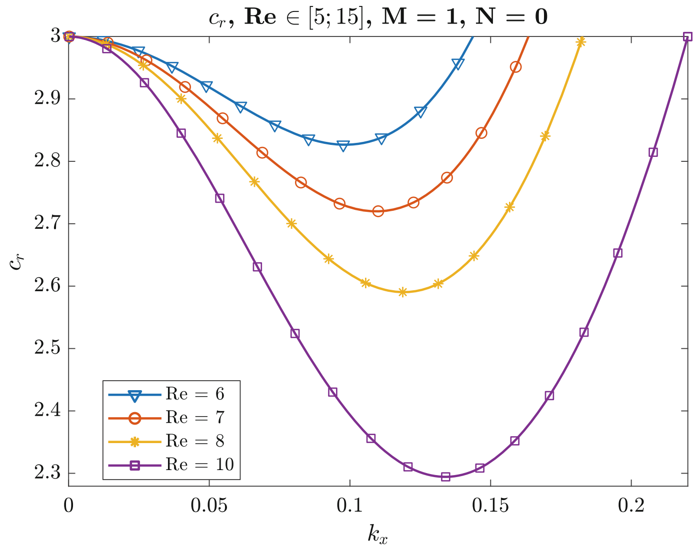

Fig. 6. Phase velocity of liquid film flowing over the heated surface.

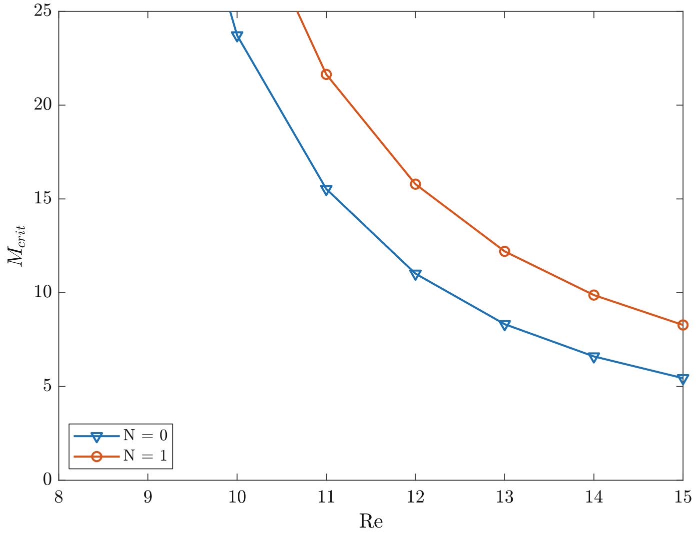

Fig. 7. Critical values of temperature gradients.

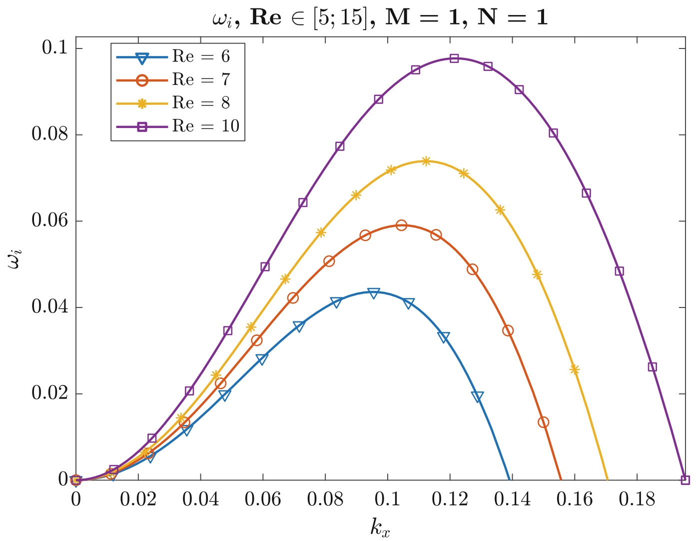

Fig. 8. Increment of liquid film with insoluble surfactants

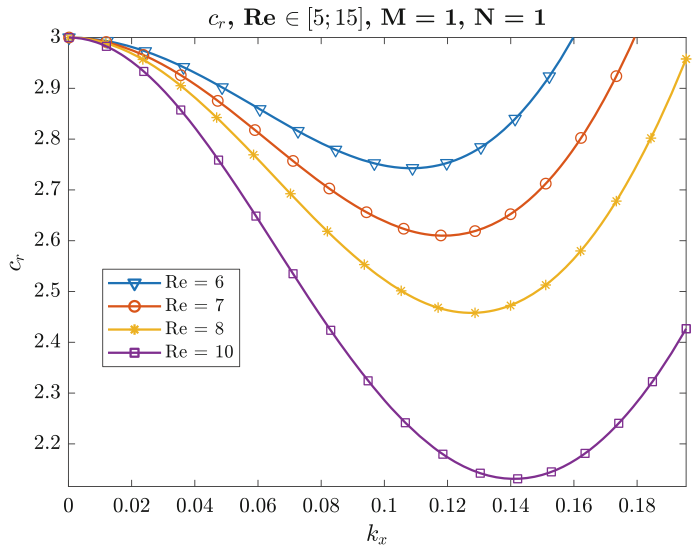

Fig. 9. Phase velocity of liquid film with insoluble surfactants

4 Conclusion

In the framework of free surface state differential Eq. (1), numerical simulation of unstable flow regimes of a vertical liquid water film at moderate Reynolds numbers is carried out.

Optimal flow regimes of the liquid film characterized by the maximum increment and the minimum phase velocity are revealed.

The destabilizing effect of temperature gradients on the wave characteristics of the liquid film was studied. Critical values of the temperature gradients that lead to destruction of film are calculated.

Presence of insoluble surfactants on the free surface of film leads to the appearance of surface viscosity forces that stabilize the film flow. Wave characteristics of the liquid film with the combined effect of temperature gradients and surface viscosity are calculated.

Results of computational experiments are aimed at improving the technologies in liquid films and operation of film devices.

The main contribution of this article is pointing out optimal liquid flow regimes. That includes adding insoluble surfactants into the liquid film in order to achieve more stable flow when liquid films are used in different heated devices.

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