Numerical simulation of the drop spreading on a horizontal plane

N A Zyuzina¹ and V V Ostapenko¹,²
¹Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia
²Novosibirsk State University, Novosibirsk, Russia
E-mail: nzyuzina1992@gmail.com

Abstract. A shallow water model of film flow is used to describe the process of a drop spreading on a horizontal plane, taking into account the liquid viscosity, heat-mass transfer and surface tension forces. To simulate this flow numerically in polar coordinates an unconditionally stable implicit difference scheme has been developed, which (in the case of evaporation) can calculate the drop spreading over a dry surface without special allocation of the drop boundary. A region of dimensionless parameters is singled out under which the evaporating droplet, as a result of surface tension forces, transforms into a circular ring before complete evaporation.

1. Introduction

The process of a liquid drop spreading over a horizontal plane is of classical interest and have been studied by various authors, since many industrial applications (lubrication, coating, painting) require the spreading of a liquid on a solid. The independent directions of investigations are a migration of liquid droplets on the solid surfaces [1], spreading of evaporating (volatile) drops [2–5], evaporation of sessile drops [6, 7], dynamic contact angles and moving contact lines [8, 9], gravity effect [10–12]. Such researches are useful in understanding of wetting phenomena [13] and for some technological and biological applications (coating, drying, spray cooling, tissue spreading, cell sorting).

In this paper, using the hydrodynamic approach [9,14,15], we apply a shallow water model of film flow to describe the process of a drop spreading on a horizontal plane, taking into account the liquid viscosity, heat-mass transfer and surface tension forces. To simulate this flow numerically in polar coordinates an unconditionally stable implicit difference scheme has been developed, which (in the case of evaporation) can calculate the drop spreading over a dry surface without special allocation of the drop boundary. A region of dimensionless parameters is singled out under which the evaporating droplet, as a result of surface tension forces, transforms into a circular ring before complete evaporation.

2. Mathematical Model

Let us consider a viscous incompressible fluid flowing at a velocity \( \mathbf{u} = (u,v,w) \) along the horizontal plane \( \alpha \), which in the Cartesian coordinate system \( \{x,y,z\} \) is given by the equation \( z = 0 \). The fluid is subjected to the gravity force, which generates an acceleration \( \mathbf{g} = (0,0,-g) \) directed vertically downward. We assume that in the cylindrical coordinate system \( \{r,\alpha,z\} : x = r \cos \alpha, y = r \sin \alpha \) the horizontal velocity components are determined by
formulas \( u = q \cos \alpha, \ v = q \sin \alpha \), where the modulus \( q = \sqrt{u^2 + v^2} \) of the horizontal velocity vector \( v = (u, v) \), as well as other scalar flow parameters, do not depend on the angle \( \alpha \). In this case, the fluid flow in the cylindrical coordinate system is described by the following Navier-Stokes, continuity and thermal conductivity equations:

\[
\begin{align*}
q_t + q q_r + w q_z + p_r &= \mu \left( q_{rr} + q_{zz} + q_r/r - q/r^2 \right), \\
w_t + q w_r + w w_z + p_z + g &= \mu \left( w_{rr} + w_{zz} + w_r/r \right), \\
q_r + w_z + q/r &= 0, \\
\theta_t + q \theta_r + w \theta_z &= a \left( \theta_{rr} + \theta_{zz} + \theta_r/r \right),
\end{align*}
\]

where \( p \) is the specific pressure, \( \theta \) is the temperature, \( \mu \) is kinematic viscosity and \( a \) is thermal diffusivity.

As the boundary conditions for the liquid, we set the adhesion condition on the plane \( \alpha \):

\[
q(r, 0, t) = w(r, 0, t) = 0,
\]

the flow potentiality, the kinematic and dynamic conditions on the free surface \( z = h \):

\[
(q_z - w_r) |_{z=h} = 0,
\]

\[
\gamma (h_t + q h_r - w) = \lambda (\theta_z - h_r \theta_r) / \varphi, \quad \varphi = \sqrt{1 + (h_r)^2}, \quad z = h,
\]

\[
p = 2 \mu \left( (h_r)^2 q_r + w_z - h_r (w_r + q_z) \right) / \varphi^2 - \sigma (h_{rr}/\varphi^2 + h_r/(r \varphi^2)), \quad z = h,
\]

where \( h = h(r, t) \) is the liquid depth, \( \gamma \) is the latent heat, \( \lambda \) is the thermal conductivity, \( \sigma \) is the surface tension coefficient. The boundary values for the temperature are given by the formulas

\[
\theta(r, 0, t) = \theta_0, \quad \theta(r, h, t) = \theta_1, \quad \theta_0, \theta_1 = const.
\]

Let us introduce the following dimensionless variables

\[
\begin{align*}
r_* &= \frac{r}{L}, \quad z_* = \frac{z}{H}, \quad t_* = \frac{t}{T}, \quad h_* = \frac{h}{H}, \quad q_* = \frac{q}{Q}, \quad w_* = \frac{w}{W}, \quad p_* = \frac{p}{P}, \quad \theta_* = \frac{\theta}{\Theta},
\end{align*}
\]

\[
\begin{align*}
g_* &= \frac{g}{G}, \quad \mu_* = \frac{\mu}{M}, \quad a_* = \frac{a}{A}, \quad \lambda_* = \frac{\lambda}{\Lambda}, \quad \gamma_* = \frac{\gamma}{\Gamma}, \quad \sigma_* = \frac{\sigma}{S},
\end{align*}
\]

where \( L, H, T, Q = L/T, W = H/T, P, \Theta, G, M, A, \Gamma, \Lambda \) and \( S \) are characteristic wave length, depth, time, horizontal and vertical velocity, pressure, temperature, gravity acceleration, viscosity, thermal diffusivity and conductivity, latent heat and surface tension respectively. Eq. (3) written in dimensionless variables (9), (10) remains unchanged; Eq. (1), (2), (4) and boundary condition (6)–(8) become

\[
\begin{align*}
\epsilon T \left[ Q^2 (q_t + q q_r + w q_z) + P p_r \right] &= M \mu \left[ q_{zz} + \varepsilon (q_{rr} + q_r/r - q/r^2) \right], \\
\epsilon T (w_t + q w_r + w w_z) + P p_z + G H g &= M \mu \left[ w_{zz} + \varepsilon (w_{rr} + w_r/r) \right], \\
\epsilon L^2 (q_r + q r_t + w z_r) &= T A a \left[ q_{zz} + \varepsilon (q_{rr} + q_r/r) \right], \quad (q_z - \varepsilon w_r) |_{z=h} = 0, \\
\epsilon L^2 \gamma (h_t + q h_r - w) &= T \Theta \Lambda \lambda \left( \theta_z - \varepsilon h_r \theta_r \right) / \varphi, \quad \varphi = \sqrt{1 + \varepsilon (h_r)^2}, \quad z = h, \\
P p &= \frac{2 M \mu}{T \varphi^2} \left( w_z + \varepsilon (h_r)^2 q_r - h_r (q_z + \varepsilon w_r) \right) - S H \sigma \frac{\lambda}{L^2 \varphi^2} \left( h_{rrr} + \varphi h_r \right), \quad z = h,
\end{align*}
\]
where \( \varepsilon = H^2/L^2 \ll 1 \) is the small parameter of long-wave approximation [16]. Here and elsewhere the asterisk at the dimensionless variables is omitted for brevity.

Assuming that the characteristic quantities satisfy conditions

\[
M = O(\varepsilon), \quad \varepsilon Q^2 = o(\varepsilon), \quad P = ML^2/(TH^2) = GH = SH/(L^2), \quad \Gamma H^2 = T\Theta = \Rightarrow \]

\[
L = \sqrt{S/H}, \quad T = ML^2/(GH^3) = MS/(GH^4) = \Gamma H^2/(\Theta L),
\]

from Eq. (11)–(16) in the long-wave approximation, we obtain

\[
p_r = \mu q_{zz}, \quad p_z + g = 0, \quad \theta_{zz} = 0, \quad (17)
\]

\[
q_z|_{z=h} = 0, \quad (h_t + gh_r - w - \lambda \theta_z/\gamma)|_{z=h} = 0, \quad (p + \sigma(rh_r)_r)|_{z=h} = 0. \quad (18)
\]

Integrating the second equation (17) with allowance for the third boundary condition (18), we have

\[
p = g(h - z) + p(h) = g(h - z) - \sigma(rh_r)_r/r, \quad z \in [0, h]. \quad (19)
\]

Integrating the first equation (17) with taking into account Eq. (19), boundary condition (5) and first boundary condition (18), we obtain

\[
q = (p_r/\mu) (z^2/2 - h z), \quad p_r = gh_r - \sigma ((rh_r)_r/r). \quad (20)
\]

Integrating the third equation (17) with allowance for the boundary condition (9), we have

\[
\theta_z = b, \quad \theta = bz + \theta_0, \quad b = (\theta_1 - \theta_0)/h, \quad (21)
\]

Integrating the continuity equation (3) with respect to \( z \) from \( z = 0 \) to \( z = h \) taking into account Eq. (20), (21) and second boundary condition (18), we obtain differential equation

\[
\frac{1}{3r} \left[ \alpha_1 (r h^3 h_r)_r - \alpha_2 \left( r h^3 \left( \frac{(r h_r)_r}{r} \right)_r \right) \right] + \frac{\beta}{h} \quad (22)
\]

for calculating the film thickness \( h(r, t) \), where \( \alpha_1 = g/\mu, \ \alpha_2 = \sigma/\mu \) and \( \beta = \lambda(\theta_1 - \theta_0)/\gamma \). We note that Eq. (22) can be regarded as a particular case of the equation derived in [17]. Multiplying Eq. (23) by \( 2h \), introducing the notation \( \eta = h^2 \) and taking into account that \( h_r = \eta_r/(2h) \), we have

\[
\eta_t = \frac{h}{3r} \left[ \alpha_1 (r h^2 \eta_r)_r - \alpha_2 \left( r h^3 \left( \frac{1}{r} \left( \frac{r \eta_r}{h} \right)_r \right) \right)_r \right] + 2\beta. \quad (23)
\]

Performing differentiation in the second term in square brackets, we find

\[
\eta_t = \frac{h}{3r} \left[ \alpha_1 (r h^2 \eta_r)_r - \alpha_2 (k_1 \eta_r - k_2 \eta_{rrr} + k_3 \eta_{rrrr} + k_4 \eta_{rrrrr}) \right] + 2\beta, \quad \eta = h^2, \quad (24)
\]

where

\[
k_1 = \frac{h^2}{r^2} + (h_r - 2h/r) h_r + (3r h_r - 2h) h_{rr} - r h_{rrr}, \quad k_2 = \frac{h^2}{r} + h h_r + r h_{rr}, \quad k_3 = 2h^2, \quad k_4 = h^2.
\]

The advantage of Eq. (24), in comparison with Eq. (22), is that it lacks a singularity at \( h = 0 \), which makes it possible to simulate the propagation of a droplet over a dry surface without specifying its boundary. For Eq. (24), we set the following initial-boundary value problem

\[
h(r, 0) = \left\{ \begin{array}{ll} \sqrt{9 - r^2}, & 0 \leq r \leq r_0, \\
\frac{\sqrt{9 - r^2}}{h_0}, & r_0 \leq r \leq r_1, \end{array} \right. \quad r_0 = \frac{\sqrt{9 - h_0^2}}{h_0}, \quad r_1 = 20, \quad (25)
\]

\[
h_r(0, t) = \eta_{rrrr}(0, t) = h_r(r_1, t) = h_{rrrr}(r_1, t) = 0, \quad (26)
\]

which simulates the spreading of a drop over the residual layer of the initial thickness \( h_0 \leq 1 \).
3. Numerical simulation
Figures 1–4 show the results of numerical simulation of the problem (24)–(26) by an implicit, unconditionally stable finite-difference scheme, in the implementation of which a five-point sweep and nonlinearity iterations were applied. The calculations were performed on a rectangular finite-difference grid with parameter $\alpha_1 = 1$. The dashed line in figures shows the initial position of the drop and solid lines show its free surface at four subsequent times. Figure 1 corresponds to the condensation at $\beta = 1$, parameter $\alpha_2 = 1$ and the initial thickness of the residual layer $h_0 = 0.5$. Figure 2–4 correspond to the evaporation at $\beta = -1$ and $h_0 = 1$. The calculations shown in Figure 2 were carried out with the parameter $\alpha_2 = 0$, in Figure 3 – with $\alpha_2 = 1$ and in Figure 4 – with $\alpha_2 = 5$.

![Figure 1](image1.png)

**Figure 1.** Numerical simulation of a drop spreading in the case of condensation at $\beta = 1$ with $\alpha_1 = \alpha_2 = 1$ at the following times: $t = 0.2$ (line 1), $t = 0.5$ (line 2), $t = 1$ (line 3), $t = 2$ (line 4).

![Figure 2](image2.png)

**Figure 2.** Numerical simulation of a drop spreading in the case of evaporation at $\beta = -1$ with $\alpha_1 = 1$, $\alpha_2 = 0$ at the following times: $t = 0.3$ (line 1), $t = 0.47$ (line 2), $t = 1.3$ (line 3), $t = 1.8$ (line 4).

![Figure 3](image3.png)

**Figure 3.** Numerical simulation of a drop spreading in the case of evaporation at $\beta = -1$ with $\alpha_1 = \alpha_2 = 1$ at the following times: $t = 0.3$ (line 1), $t = 0.5$ (line 2), $t = 1.7$ (line 3), $t = 1.93$ (line 4).

![Figure 4](image4.png)

**Figure 4.** Numerical simulation of a drop spreading in the case of evaporation at $\beta = -1$ with $\alpha_1 = 1$, $\alpha_2 = 5$ at the following times: $t = 0.3$ (line 1), $t = 0.5$ (line 2), $t = 1.1$ (line 3), $t = 1.6$ (line 4).

It follows from these calculations that for a finite value of the parameter $\alpha_2$ responsible for the surface tension, a sequence of damped waves is formed on the surface of the residual layer.
over which the drop spreads (only the first downward wave is clearly visible in Figures 1,3,4). In the case of condensation, the increasing residual layer gradually absorbs these waves and at the time $t \approx 1$ (line 3 in Figure 1) the surface of the residual layer becomes monotonous. In the case of evaporation, the amplitude of these waves gradually increases, which leads to the appearance of a sequence of decreasing annular film layers before the complete evaporation of the residual layer. Only the first annular film layer from this sequence is clearly visible in Figures 3,4 (line 2 in these figures). The calculations shown in the Figure 3 also revealed the following interesting fact: the surface tension at $\alpha_2 = 1$ forms a hollow at the drop top which increases in time (line 3) and leads to the transformation of the drop into an annular film layer (line 4) before its complete evaporation.

4. Conclusion
This article proposes a shallow water model of the film flow for describing the process of a drop spreading on a horizontal plane, taking into account the gravity acceleration, liquid viscosity, heat-mass transfer and surface tension forces. The main advantage of this model is that the resulting differential equation (24) describing the evolution of the thickness $h$ of a liquid film has no singularity at $h = 0$ which allows to simulate the propagation of a droplet over a dry surface without specifying its boundary. This, in particular, makes it possible to numerically determine the values of the triple angle at the gas-liquid-solid interface without additional heuristic assumptions.

Acknowledgments
The authors are grateful to Prof. V.V. Kuznetsov for useful comments made during the discussion of this work. The work was supported by the Russian Science Foundation (grant No. 15-19-10025).

References
[1] Smith M K 1995 J. Fluid Mech. 294 209
[2] Potash M and Wayner P C 1972 J. Heat Mass Transfer 15 1851
[3] Ruiz O E and Black W Z 2002 J. Heat Transfer 124 855
[4] Ajaev V S 2005 J. Fluid Mech. 528 279
[5] Strotos G, Gavaises M, Theodorakakos A and Bergeles G 2008 Int. J. Heat Mass Transfer 51 1516
[6] Hu H and Larson R G 2005 Langmuir 21 3963
[7] David S, Seifiani K and Tadrist L 2007 Colloids Surf. A Physicochem. Eng. Asp. 298 108
[8] Greenspan H P 1978 J. Fluid Mech. 84 125
[9] Dussan V 1979 Annu. Rev. Fluid Mech. 11 371
[10] Shikhmurzaev Y D 1997 Phys. Fluids 9 266
[11] Reznik S N and Yarin A L 2002 Int. J. Multiph. Flow 28 1437
[12] Bartashevich M V, Kuznetsov V V and Kabov O A 2010 Micrograv. Sci. Technol. 22 107
[13] Gennes P G 1985 Rev. Mod. Phys. 57 827
[14] Tanner L H 1979 J. Phys. D Appl. Phys. 12 1473
[15] Voinov V V 1995 Int. J. Multiph. Flow 21 801
[16] Friedrichs K O 1948 Comm. Pure Appl. Math. 1 109
[17] Kabova Yu, Kuznetsov V V and Kabov O 2014 Interfacial Phenom. Heat Transfer 2 85