Numerical Modelling of Liquid Film Spreading Dynamics over Smooth Vertical Surface under Isothermal Conditions

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Abstract. The paper presents numerical modelling of the liquid film spreading dynamics of the R21 (mol. fraction: 0.9) and R114 refrigerants mixture. We considered an outer flow along a round vertical cylinder at Reynolds number of 104 and various contact angles. The simulation was performed in OpenFOAM software on the basis of the volume of fluid (VOF) method. We have shown that the wetting front deforms at wetting angles of 30 and 50 degrees, and regular jets form. At the same time, it was demonstrated that at the wetting angle of 10 degrees the spreading front has practically a flat shape, but one may see some regular thickenings of the liquid film along the contact line of the front.

1. Introduction
Falling liquid films, being an effective means of interfacial heat and mass transfer, are used in various technological processes, including: evaporation, condensation, distillation, adsorption, desalination, etc. [1]. Nowadays, when there is an increasing number of studies devoted to the enhancement of heat transfer at pool boiling of liquids on modified surfaces [2, 3], it is also necessary to continue to develop studies of heat and mass transfer and hydrodynamics in the film flow of liquids on enhancing surfaces. This, among other things, will facilitate the transition from traditional submersible heat exchangers to more efficient film heat exchangers, creation of more advanced mass transfer columns, etc.

Available research suggests a significant effect of surface structure on film flow dynamics and heat transfer rate [4-6], modern research on the influence of wettability carried out under pool boiling conditions shows the significant effect of wetting on the heat transfer enhancement [7-9]. However, at the moment there are only a few works on modeling the flow of low-viscosity fluids over heat-transfer surfaces of complex geometry or different wettability in the literature [6]. Most of the computational works relate to the simulation of fluid flow over bundles of smooth horizontal tubes, since tube bundles are the main structural elements of promising film heat exchangers. So, for example, the authors of [10, 11] provided the 2- and 3D simulation of flow behavior and film distribution outside a smooth horizontal tube.

The authors of the mentioned above work [6] studied flow characteristics of a liquid film flowing over a smooth vertical cylinder and vertical cylinder with transverse ribbing. The Reynolds number ranged from 10 to 1121. The binary mixture of R21 and R114 refrigerants is used as the working liquid. To capture dynamic characteristics and spatial distribution of the liquid film flow, 3D simulations were carried out. It was shown that surface tension has a great influence on the flow pattern, while the inlet width has no effect on the film flow parameters at the steady-state flow regime.
For both the smooth surface and the ribbed one, flow rates have great effects on wettability, film velocity and film thickness. The simulation also showed that a ribbed surface structure hinders the liquid film movement, reflected in a lower velocity and a larger film thickness as compared to the smooth surface. Lateral movement of a film can also be observed at the ribbed surface.

The goal of this investigation is the numerical modeling of the liquid film spreading dynamics over the preliminarily non-wetted surface at variable wetting angle.

2. Flow configuration and modelling approach
We considered the liquid film spreading of the R21 (mol. fraction: 0.9) and R114 refrigerant mixture over the quarter of the round vertical cylinder with radius of 25 mm and height of 90 mm (Figure 1). The modelling volume was limited by the imaginary outer cylinder with radius of 26 mm. An area with the initial liquid film thickness \( \delta = 0.25 \text{mm} \) and initial liquid velocity \( V_{i0} = -0.1 \text{ m/s} \) was set on the upper horizontal plane. Taking into account the properties of the above pointed refrigerants mixture, Reynolds number was \( Re = \Gamma / \nu = V_{i0} / \delta / \nu = 104 \), where \( \Gamma \) is the liquid flow rate per unit of film width and \( \nu \) is the kinematic viscosity. We applied constant properties of the refrigerant mixture in liquid and gas phases.

![Figure 1. Diagram of the flow considered.](image)

2.1. Equations and boundary conditions
The simulation was performed in OpenFOAM software on the basis of the volume of fluid (VOF) method. We used solver «compressibleInterFoam» that consists of the conservation laws of mass, momentum and energy as well as a transport equation for the liquid volume fraction. The energy equation is omitted below since we considered isothermal flow without the Marangoni effect:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) &= 0, \\
\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) - \nabla \cdot (\mu \nabla U) &= \sigma \kappa \nabla \alpha - g \cdot X \nabla \rho - \nabla P_d,
\end{align*}
\]
where $U$ is a velocity vector, $\sigma$ is the surface tension coefficient, $\kappa$ is the curvature of the interface, $P_d$ is the dynamic pressure and $X$ is the position vector;

$$\frac{\partial \alpha}{\partial t} + U \cdot \nabla \alpha + \nabla \cdot U, \alpha (1 - \alpha) = 0$$

(3)

where $\alpha$ is the volume phase fraction coefficient. Values of $\alpha = 1$ correspond to mesh cells fully filled with liquid; a mesh cell contains only gas phase at $\alpha = 0$, while intermediate values of this coefficient mean the presence of the interface within a mesh cell.

The volume fraction near the wall has a correction through the wetting angle:

$$\cos \theta = \frac{\nabla \alpha_{corr}}{\left| \nabla \alpha_{corr} \right|} \cdot n_w,$$

(4)

where $\nabla \alpha_{corr}$ is the corrected volume fraction gradient, $n_w$ is the unity vector normal to the surface.

The interaction between velocity and pressure was established by the PISO algorithm. Also, we considered the laminar regime for both phases and constant liquid density.

The following conditions were applied at borders of the modeling volume:

- $y = 0.09: U = (0;V_0;0), \alpha = 1, \delta \rho / \delta n = 0$ represent initialization of the liquid film,
- $x^2 + z^2 = R_{cyl}^2: U = (0;0;0), \alpha = 0, \theta = const, \delta P / \delta n = 0$ represent the solid surface of the cylinder,
- $x^2 + z^2 = R_{cyl}^2$ and $y = 0$:

are at free borders of the modeling volume.

At the initial time ($t = 0$), the modeling volume had the following parameters: $U = (-0.005,0,0)$, $\alpha = 0$, $P = 2 \times 10^5 Pa$, $T = 300 K$. The initial continuous contact line was set near the upper inlet of liquid.

Figure 2. Parts of Mesh in ZX-view (left) and XY-view (right).
2.2. Mesh
To perform the simulation we created a hexagonal mesh with number of cells of 20×500×400 (x×y×z) and compression to the solid surface (Figure 2). The time step did not exceed Δt = 2×10⁻⁵ s. The mesh has the following characteristics: maximal aspect ratio of 8.83, minimal cell volume of 3.68×10⁻¹³ m³, maximal cell volume of 2.92×10⁻¹² m³, maximal non-orthogonality of 3.91×10⁻⁶, average non-orthogonality of 0, and maximal skewness of 0.0048. Initially, we performed the simulation with 100 cells in the z-direction that led to decay of continuous liquid front on small drops with the cell size. Number of cells in x and y directions has no such strong effect on the liquid film spreading.

3. Results
Figure 3 demonstrates the dynamics of the wettability front on time at contact angle θ = 10°. We visualized the film through the volume phase fraction coefficient α. Figure 3a shows the moment with arising irregularities on the liquid film front (t = 0.38s). Figure 3b shows further spreading of the film front. Some increase of liquid front irregularities is seen. They keep on a weak increase up to the low border of the model volume (Figure 3c, t = 0.44s), but ones do not form jets under the considered conditions. On the background of the liquid front deformation, it is worth noting an existing of regular film thickening (liquid rolls) along the contact line.

Figure 4 illustrates the evolution of the liquid film front at θ = 30°. Irregularities arise at the film front at t = 0.23s from the initialization of the liquid film flow over cylinder (Figure 4a). Further, they form 7 rivulets (liquid jets) (Figure 4b) that are kept while interjet zones reach the low border of the modeling volume at t = 0.48s (Figure 4c). Parameters of these irregularities may be described roughly by the Rayleigh–Taylor instability. Our analysis demonstrates that interjet distances of 0.004 m and 0.0068 m are of the same order with the critical wave-length 2πΛ = 0.007 m and the most dangerous wave-length √32πΛ = 0.012 m. Li et al. [6] made similar conclusions for the considered refrigerants mixture at Re = 280. The paper [12] reports on the detailed comparative analysis of characteristic sizes
of such regular structures with parameters of Rayleigh–Taylor instability for nitrogen falling films in the regimes of evaporation and boiling.

Figure 4. Front view (ZY) of Freon film at $\theta = 30^\circ$ and $Re=104$.

Figure 5. Front view (ZY) of Freon film at $\theta = 50^\circ$ and $Re=104$. 
Figure 5 shows the film spreading dynamics of the refrigerants mixture at $\theta = 50^\circ$. It is seen that instabilities in the liquid front arise significantly earlier ($t = 0.20s$) and at a shorter distance from the liquid inlet (Figure 5a) than those for the flow with $\theta = 30^\circ$. At that, interjet distances increase up to 0.0045$m$ and 0.0082$m$, respectively, and the number of liquid jets decreases to 6 (Figure 5b). Also, the increase of contact angle increases the time, at which the film front in the interjet zones reaches the low border of the modeling volume (Figure 5c, $t = 0.63s$).

4. Conclusions
Numerical modelling of the liquid film spreading over the round vertical cylinder demonstrated that the wettability angle has a significant effect on the dynamics of liquid film propagation. At small contact angle of 10 degrees, the liquid front deformation is weakly expressed by some thickening of the liquid film in the front locality. At contact angles of 30 and 50 degrees, one can see the pronounced formation of the regular rivulets (liquid jets) at the wettability front. The increase of contact angles increases the velocity of jets and decreases the velocity of liquid front in interjet zones. The significant deceleration of the film front in interjet zones is associated with the accumulating of the main liquid flow rate in the fast propagating jets. Also, the increase in contact angle decreases the time of arising of liquid front deformation almost twice. Distances between jets are in the range of characteristic scales of Rayleigh–Taylor instability. Thus, dynamics of the wettability front of dry surface depends significantly on the contact angle.

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