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Simulation of Wetting of a Solid of Revolution by Viscous Liquid

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Abstract. Accounting for the nature of interaction between the solid and liquid phases, one can create a material with predetermined wetting characteristics. After design of such materials, proper verification is needed. Since experimental verification is usually resource-consuming, this problem can be efficiently solved via computer simulation. In this work, we used the phase field method to simulate wetting of a solid of revolution. The adequacy of the formulated model is shown, and the problems of numerical stability are discussed.

PROBLEM STATEMENT

The statement of the problem is shown in Fig. 1 where a ring-shaped liquid film is located on a solid surface at the initial time. We consider a non-stationary process of wetting of a substrate. The liquid phase wets the surface of the substrate and spreads along it under action of the tension forces. The problem is symmetric about the axis of rotation of the disk. Thus, to obtain a solution of the three-dimensional bulk problem, one can simulate the wetting in the cross section of the disk only (Fig. 2) and integrate this solution over the angular coordinate. The thermophysical properties of the liquid, gas and solid phases can be used then to solve the dynamic contact problem for a specific liquid-solid pair.

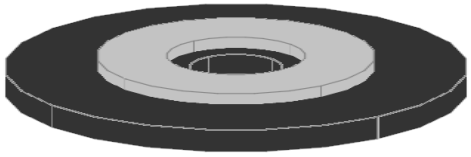

FIGURE 1. The modeled geometry in 3D. The liquid film (grey color) is located on the upper surface of a solid disk (black color) with a hole.

Several assumptions have been made that (i) the densities and viscosities are constant, (ii) the surface of the substrate is smooth, (iii) the viscosity of the gaseous medium is equal to the viscosity of the liquid. These assumptions are justified as follows. The surface of the substrate can be considered smooth, since it is always possible to calculate the problem for such local regions in which the radius of roughness is much smaller than the average thickness of the film. The equal viscosities of the gas and liquid were chosen in order to simplify the process of mathematical modeling. Since the viscosity of gases is much lower than the viscosity of liquids, turbulence can occur in the gas environment. This turbulence has almost no effect on the dynamics of the liquid phase on the solid surface. Increasing the viscosity of the gas leads to decrease of the Reynolds number in the gas. Thus, there are no vortices in it, which speeds up calculations.

All solids of revolution are symmetric about their axis of rotation. Therefore, to obtain a solution to the three-dimensional problem, one only needs to simulate wetting in the cross section of the body and integrate this solution over the angular coordinate. Figure 2 shows the cross section for a case where the fluid wets the disc with a hole.

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Using the known thermophysical properties of the liquid, gas phase and solid surface, it is possible to solve the dynamic contact problem for a specific pair of contacting media.

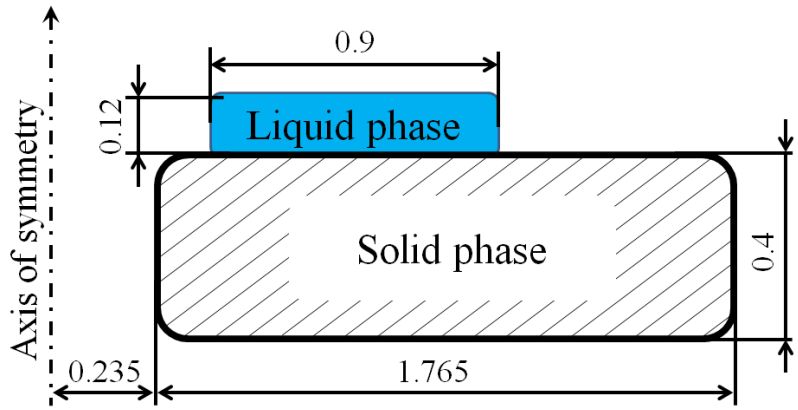

FIGURE 2. Geometry of the modeled problem in 2D. The liquid film is located on the upper surface of a disk with a hole. The dimensions are given in mm.

MODEL

The mathematical model used in this paper is based on the phase field theory combined to the Navier-Stokes equations for multiphase flows in incompressible fluids. The governing equations (1)–(3) and the boundary conditions (4)–(10) are as follows [1–4]:

$$\frac{\partial \varphi}{\partial t} + (\vec{u} \cdot \nabla)\varphi = \nabla \cdot (B \nabla M), \tag{1}$$

$$M = \frac{\partial f}{\partial \varphi} - \kappa \nabla^2 \varphi, \tag{1a}$$

$$f(\varphi) = -p_0 + \Delta f(\varphi); \Delta f(\varphi) = \frac{1}{4} W \varphi^2 (1-\varphi)^2, \tag{1b}$$

$$\rho(\varphi)\left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} \right) = -\nabla p + \nabla^2 (\mu(\varphi)\vec{u}) + \rho(\varphi)\vec{g} + M \nabla \varphi, \tag{2}$$

$$\nabla \cdot \vec{u} = 0, \tag{3}$$

where φ is the phase field variable, t is time, $\vec{u}$ is flow velocity, B is the mobility of the phase field, M is the chemical potential, f is the free energy density, κ is the gradient coefficient, W is the height of the double-well potential barrier (between the liquid and gas phases), p_0 is the gas pressure in the upper node, p is pressure, g is the gravitational acceleration, ρ is the fluid density, and μ is the dynamic viscosity of fluid. Equation (1) determines motion of the phase field. Equations (1a) and (1b) determine the chemical potential and the Helmholtz free energy density correspondingly. Equations (2-3) are the Navier-Stokes equations for incompressible fluid.

On the surface, the slip boundary condition is set as:

$$\vec{u} = 0. \tag{4}$$

At the boundaries of the computational domain, zero flux of the phase field is set:

$$\nabla \varphi \cdot \vec{n} = 0. \tag{5}$$

At the boundaries of the computational domain and on the surface of the solid, zero flow of the chemical potential is defined:

$$\nabla M \cdot \vec{n} = 0. \tag{6}$$

At the wetted boundary, a non-stationary diffusion-type condition is set [2]. It guarantees the absence of convection and at the same time ensures that the contact point diffusively moves along the wall due to wetting:

$$\frac{D\varphi}{Dt} = \frac{\partial\varphi}{\partial t} = -b(\kappa\vec{n}\cdot\nabla\varphi + \gamma'(\varphi)(\varphi-\varphi^2)), \tag{7}$$

where γ' is the difference between the "solid/liquid" and "solid/gas" surface tensions, b is the contact mobility of the phase field. This condition is a phase-field analogue to the balance of surface energies at the contact point [2]. The zero viscosity tensor at the boundaries of the computational domain means the absence of fluid along the open boundary:

$$\tau = 0. \tag{8}$$

In a single node of the computational domain, the fixed pressure is set:

$$p = p_0. \tag{9}$$

The initial condition at $t = 0$ corresponds to a liquid at rest:

$$\vec{u} = 0, \varphi = \varphi_0(\vec{r}), \tag{10}$$

where $\vec{r}$ is the radius vector. To solve this problem, the finite element method was used in the Galerkin's formulation. The computations have been performed using the COMSOL Multiphysics software, version 3.5a, licence No. 1056903.

PHYSICAL PROPERTIES

Table 1 provides the physical properties that were used in calculations. We note that the viscosity of gas was chosen artificially equal to the viscosity of liquid in order to reduce the Reynolds number in the gas phase.

TABLE 1. Physical properties of water used to solve the problem of wetting over the hydrophilic surface

Parameter	Value
Density of liquids	1000 kg/m^3
Viscosity of liquids	0.001 kg/(m·s)
Density of gas	1.184 kg/m^3
Viscosity of gas	0.001 kg/(m·s)
Liquid/gas surface tension	0.072 N/m
Solid/liquid surface tension	0.0008 N/m
Solid/gas surface tension	0.0727 N/m
Equilibrium contact angle	3.02°

TEST RUNS

We decided to test the model using a simple geometry that is shown in Fig. 3. This geometry corresponds to a big circular plate with vertical walls (similar to the shape of a Petri dish).

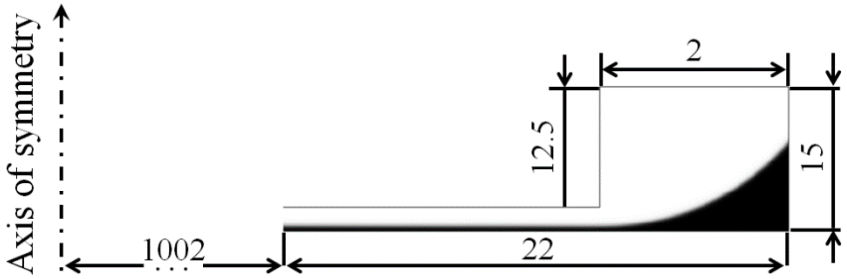

FIGURE 3. Simple geometry that was used in test runs. All dimensions are given in mm.

To verify the adequacy of the formulated model, Washburn's law was used, which establishes a relation between the meniscus height h and time t: $h \sim t^{1/n}$, where n is the power. Figure 4 shows that the dependence of the meniscus

elevation height (along the right vertical boundary) on time is a power function, which is consistent with Washburn's law.

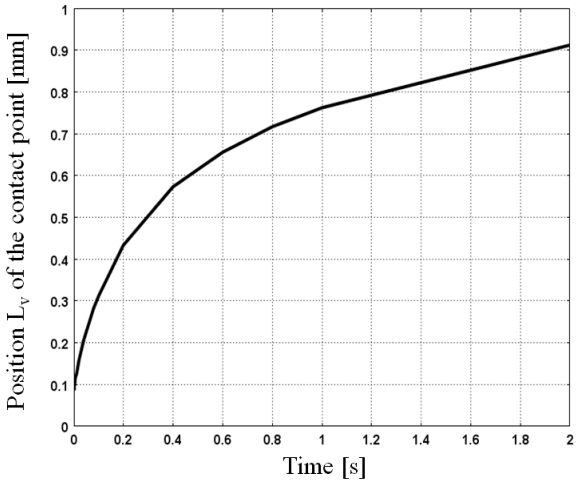

FIGURE 4. Dependence of the contact point position on time. Here L_v is the vertical position of the contact point in mm.

To determine *n*, we plotted the dependence of the position of the contact point on time on the logarithmic scale (Fig. 5). The obtained value of *n* is approximately $n \approx 3$, which is also consistent with Washburn's law.

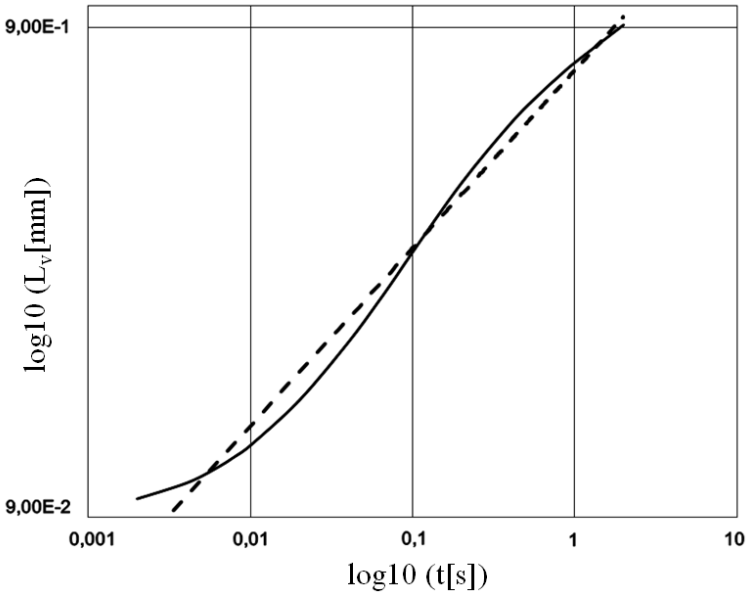

FIGURE 5. Kinetics of motion of the contact point on the logarithmic scale. The solid line corresponds to the calculated results, the dashed line yields an approximation of the solution.

MESH PARAMETERS

The distribution of finite element's sizes is shown in Fig. 6. We used a space-adaptive quadrilateral mesh with a small growth coefficient in the range between 1.0 and 1.1. It is found that such grid ensures better calculation of variable's gradients than the commonly used triangular grid. The mesh contained 13407 elements and 410436 degrees of freedom.

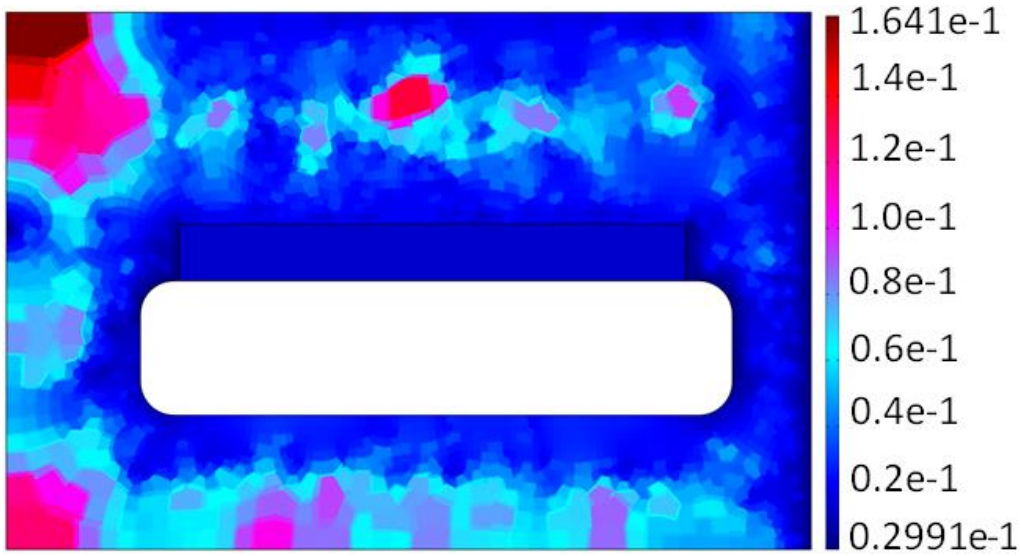

FIGURE 6. Distribution of sizes of the finite elements. The dimensions are given in mm.

RESULTS AND DISCUSSION

The results of calculations are presented in Fig. 7. The simulated positions of the "liquid-gas" interface correspond to the dynamics of water. In the case of a small (< 10°) equilibrium angle as well as provided that the mass of the liquid is small, the liquid completely surrounds the body and forms a film on its surface.

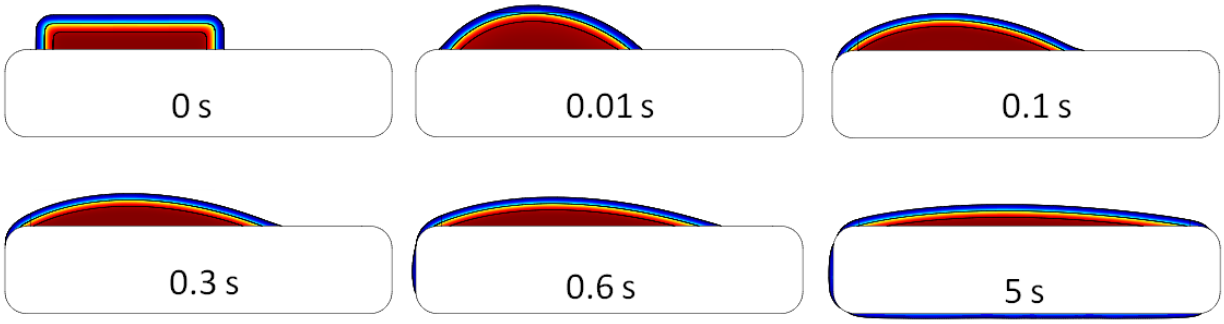

FIGURE 7. Dynamics of the wetting process. The time is given in seconds.

The main difficulties in modeling of problems in the cylindrical coordinates are due to oscillations of the solution at the initial time $t = 0$. These oscillations appear at the phase-field interface owing to coarse interpolation of the smooth phase field variable on the finite element mesh. Another problem is singularity at r=0, where r is the radial coordinate. In the model, it appears since the governing PD equations contain $1/r^n$ terms.

The problem with singularity at $r = 0$ can be solved by multiplying the equations with $1/r^n$ terms by r^n. This is possible when solving the problem with the Galerkin method. In this method, minimizing the residuals is not affected by such operations. The problem of oscillations of the initial solution can be solved by tuning the mesh. The initial distribution area should contain the mesh with equal finite elements. We have found that the transition layer in φ should contain at least 3 elements.

The model suggested in this work extends the phase-field model developed in [4] to the cylindrical formulation. The stability of the suggested solution is confirmed. It is shown that qualitative description of wetting processes by this model is adequate. The condition on numerical stability of the solution in terms of the mesh parameters is found. Further work on the model involves calibrating of the model, reconciling with experiments, and creating a computer code.

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REFERENCES

1. D.M. Anderson, G.B. McFadden and A.A Wheeler, Annual Rev. of Fluid Mechan. **30**, 139–165 (1998).
2. D. Jacqmin, J. of fluid mechan. **402**, 57–88 (2000).
3. H. Fu, F. Dong, D.P. Sekulic, S.Dj. Mesarovic and M. Krivilyov, "Surface tension driven kinetics of the triple line of a liquid metal free surface" in *ASME 2013 Int. Mechan. Engineer. Congr.s and Exposit.*, proceedings of International Mechanical Engineering Congress and Exposition 7A, pp. 13–21 (2013).
4. M. Dehsara, H. Fu, S. Dj. Mesarovic, D.P. Sekulic and M. Krivilyov, Theoret. and Appl. Mechan. **44**, 189–214 (2017).
5. M.D. Krivilyov, S.Dj. Mesarovic and D.P. Sekulic, J. of Mater. Sci. **52**, 4155–4163 (2017).