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NUMERICAL MODELING OF CAPILLARY HYSTERESIS

D. V. Gil' and O. V. Dikhtievskii

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The statement of the problem and result of numerical simulation of the processes occurring in the flow of a nonwetting liquid in thin capillaries of closed and open types are presented.

In studying the flow of a liquid in a capillary two interrelated hysteresis phenomena are usually distinguished. The first of them [1] characterizes the relation between the length of the liquid column in the capillary and the acting pressure P, and the second [2–5] is determined by changes in the contact angle as a function of the direction, the height of the liquid column in the capillary, the velocity of the liquid, and the capillary radius. Hysteresis of the contact angle has been studied quite adequately. In particular, it has been analyzed for the example of the motion of a drop or meniscus on a solid wall [2]. In that work the notion of some stable values of the contact angle at which the energy of a system with infinitesimal roughnesses or inclusions becomes minimum has been introduced into a model of the process. In [3] the hysteresis phenomenon was modeled in terms of a balance of forces along the solid-liquid-gas contact line with account for inclusions on the solid surface. In [4] hysteresis of the contact angle has been described by two processes: the diffusion transfer of liquid molecules through the solid substrate (this process is predominant when the dynamic contact angle is less than 120° and the rate of surface diffusion increases with increase in the dynamic contact angle) and a process associated with the motion of liquid molecules along the normal to the solid substrate (this process is predominant when the dynamic contact angle is close to 180°). At contact angles between 120 and 180° both processes take place.

The motion of a nonwetting liquid along a capillary wall can be characterized by certain distinctive features [6]. The meniscus flows onto the wall periodically with the pressure drop maintained constant. After the end of each period, the contact angle and the height of the meniscus start to increase due to supply of new amounts of the liquid. Along the line of the wetting perimeter the resistance of viscous forces (a potential barrier) exists in the bulk of the liquid flow, and therefore the base of the meniscus remains motionless until its height and the contact angle become large enough to overcome the potential barrier. Then, the liquid flows rapidly onto the capillary wall and the flow continues as long as the inertia force acts. In this case the base of the meniscus is displaced along the wall, and the contact angle and the height of the meniscus decrease to the initial values. From this point on, the processes recur cyclically.

In the general form the isothermal motion of a liquid in a thin capillary with a meniscus present can be described by the Stokes equations [7] for a Newtonian viscous incompressible liquid (in cylindrical coordinates (r, z). In the calculation, the one-dimensional system

$$\frac{\partial V_z}{\partial t} + \frac{V_z^2}{2l(t)} - \frac{\nu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V_z}{\partial r}\right) = \frac{l}{\rho l(t)} P, \tag{1}$$

was used, where $P = P_{00} - P|_{z=l(t)}$.

The presence and absence of the term $V_z^2/2l(t)$ in Eq. (1) correspond to the pressure P_{00} in the cup with the liquid and the pressure $P|_{z=0}$ at the entrance to the capillary, respectively. Both cases have been calculated. No substantial difference was observed for the given parameters, which shows that P_{00} and $P|_{z=0}$ differ only slightly from each other. The following results were obtained for the Stokes equation in form of Eq. (1).

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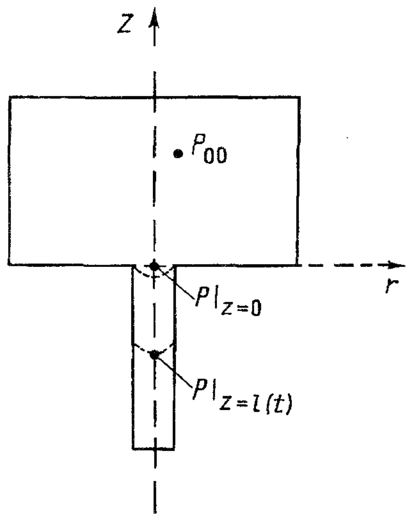

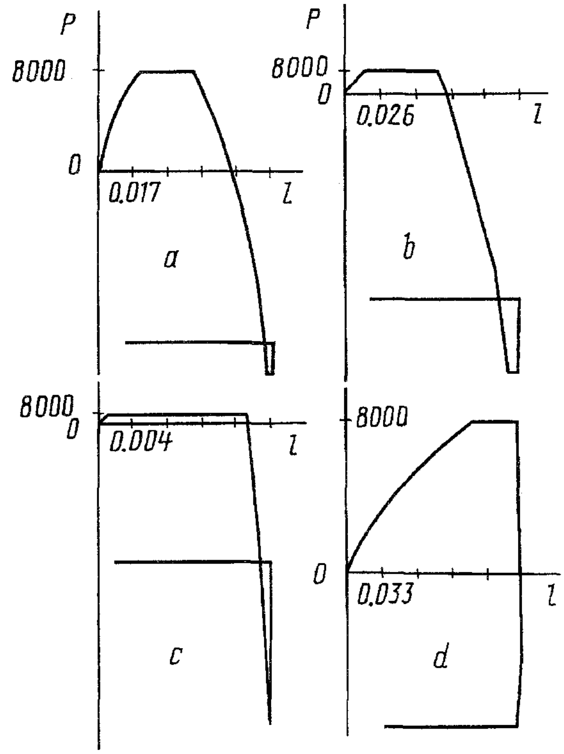

Fig. 1. Scheme of the calculation region.

Fig. 2. Plot of the pressure versus the height of a nonwetting-liquid column in capillaries: a, b, c) open capillaries with the radii $R = 10^{-4}$, 10^{-5}, and 10^{-6} m, respectively; d) closed capillary with the radius $R = 10^{-4}$ m.

The process was calculated for numerical simulation of the motion of a mercury column in a glass capillary (Fig. 1). The following initial data were used:

$$Cp_{\mathrm{Hg}} \simeq 0.136 \div 0.137 \ \ \mathrm{kJ/(kg \cdot deg)}, \quad \rho_{\mathrm{Hg}} \simeq 13507 \ \ \mathrm{kg/m^3},$$

$$\nu_{\mathrm{Hg}} \simeq 1.152 \cdot 10^{-7} \ \ \mathrm{m^2/sec}, \quad \sigma_{\mathrm{Hg}} \simeq 0.475 \ \ \mathrm{N/m}.$$

In [5] a relation is suggested for the dynamic angle θ as a function of the height of a liquid column in a capillary, the velocity of its motion, and the capillary radius. However, in the present calculations the angle θ was modeled by the simpler formula

$$V \le 0 \ \ \theta = 100^{\circ}, \quad V > 0 \ \ \theta = 140^{\circ}.$$

In studying the flow of a nonwetting liquid in a thin capillary, a model of both open and closed capillaries was considered. In the former case the process starts with the initial condition $V(t = 0) = 0$; in the latter case it is divided into two stages and the stage of reverse motion (from the bottom of the capillary) starts with the same initial condition $V = 0$.

Calculations were carried out for capillaries of various radii, and the time dependence of the external pressure was chosen so that the hysteresis loops were almost closed. The external-pressure curve is characterized qualitatively by four sections: linear load, constant pressure, linear drop, and constant pressure.

In Fig. 2a–c the pressure P is plotted versus the length of the liquid column in open capillaries of various radii, and in Fig. 2d in a closed capillary with a radius $R = 10^{-4}$ m. In all cases a linear load was produced up to a constant value ΔP.

It can be seen from a comparison of the results that for open capillaries the hysteresis loop in the lower right-hand corner is supplemented with a long narrow loop shaped like a trapezoid or a triangle. This additional loop can be ascribed to a decrease in the contact angle when the direction of the flow velocity changes, and here the Laplace pressure changes, too. The relative value of this additional loop changes from 0.105 to 0.514 for capillary radii equal to 10^{-4} and 10^{-6} m, respectively. The length of filling of an open capillary with a nonwetting liquid changes insignificantly with the capillary radius; for example, for $R = 10^{-4}$ m $l = 0.086$ m and for $R = 10^{-5}$ m $l = 0.128$ m. In closed capillaries this additional loop is absent since the liquid comes to a stop at the bottom of the capillary and its reverse motion starts with new initial conditions and the shape of the hysteresis loop turns out to depend on the shape of the external pressure curve.

In the future it is intended that modeling of the flow of a nonwetting liquid in a thin capillary include the slide effect, the energy equation, and a more accurate dependence of the contact angle on the velocity of the liquid flow, the length of the liquid column, and the capillary radius.

NOTATION

P, pressure; ρ, density; ν, viscosity coefficient; R, capillary radius; V, velocity of the liquid column; V_r, V_z, projections of the velocity V onto the r and z axes, respectively; t, time; $l(t)$, length of filling of the capillary with the liquid in the time t.

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