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PLANAR FLOWS IN NANOSCALE REGIONS

S. A. Chivilikhin[1], I. Yu. Popov[1], V. V. Gusarov[2]

[1] Saint Petersburg National Research University
of Information Technologies, Mechanics, and Optics, Saint Petersburg, Russia

[2] Saint Petersburg State Institute of Technology (Technical University),
Saint Petersburg, Russia

sergey.chivilikhin@gmail.com

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Last years, fluid flows in nano-sized domains are intensively studied [1–4] due to nontriviality of observed effects and practical importance of this part of hydrodynamics. At present, there are no general equations of nanohydrodynamics. Usually, the molecular dynamics is used for computations. As for analytical approaches, the simplest one involves introducing the slip condition at the boundary [5] together with classical hydrodynamics equations. The small scale of nanochannels gives us the possibility to use, in some cases, the Stokes approximation for motion equations [6].

In this work we apply the planar Stokes model [7] with slip boundary conditions for describing nano-flows. We have developed a method of flow calculation, which is based on the expansion of pressure in a complete system of harmonic functions. Using the pressure distribution, we calculate the velocity field and stress on the boundary. This method can be used for description of various problems of nanofluidics: hydrodynamics of nanochannels, flows along superhydrophobic surfaces, etc.

Keywords: nanofluidics, Stokes flow, nanostructure.

1. Introduction

The equations of motion in the quasi-stationary Stokes approximation and the continuity equation in the region g have the form:

$$\partial_\beta P_{\alpha\beta} = 0, \quad \mathbf{x} \in g, \tag{1}$$

$$\partial_\beta V_\beta = 0, \quad \mathbf{x} \in g, \tag{2}$$

where $P_{\alpha\beta} = -P\delta_{\alpha\beta} + \mu(\partial_\alpha V_\beta + \partial_\beta V_\alpha)$ is the Newtonian stress tensor; V_α are the components of the velocity; P is the pressure; μ is the coefficient of the dynamic viscosity, which is assumed to be constant, $\delta_{\alpha\beta}$ is the delta symbol of Kronecker. Summation over repeated indices is assumed.

We take in account four types of boundary parts: inlet, outlet, solid wall and free boundary. The total boundary γ is the union of these parts.

On the inlet we specify the velocity field

$$V_\alpha = V_\alpha^{\mathrm{in}}, \quad \mathbf{x} \in \gamma^{\mathrm{in}}. \tag{3}$$

On the outlet we use soft boundary conditions

$$\partial_n V_\alpha = 0, \quad \mathbf{x} \in \gamma^{\mathrm{out}}, \tag{4}$$

where ∂_n is the derivative along the normal to the boundary.

On the solid wall we specify slip boundary conditions

$$L\partial_n V_\tau = V_\tau, V_n = 0, \quad \mathbf{x} \in \gamma^{\mathrm{wall}}, \tag{5}$$

where V_τ and V_n are the tangent and normal components of liquid velocity on the wall, L is the slip length.

On the free boundary we assume the action of the capillary force

$$P_{\alpha\beta} n_\beta = -\sigma n_\alpha \partial_\beta n_\beta, \quad \mathbf{x} \in \gamma^{\text{free}}, \tag{6}$$

where σ is the coefficient of surface tension.

The law of free boundary evolution is determined from the condition of equality of normal velocity U of boundary and the normal component of liquid velocity at the boundary:

$$U = V_\beta n_\beta, \qquad \mathbf{x} \in \gamma^{\text{free}}, \tag{7}$$

The absence of the time derivative in the quasi-stationary motion equation (1) lets us specify the initial conditions only for the shape of the free boundary:

$$\gamma^{\text{free}}|_{t=0} = \gamma_0^{\text{free}}. \tag{8}$$

In this work we take in account two-dimensional problems only ($g \subset R^2$).

2. Calculation of the pressure and velocity with given force on the boundary

Let f_α be the force applied to the total boundary γ. Then we can write one boundary condition

$$P_{\alpha\beta} n_\beta = f_\alpha, \quad \mathbf{x} \in \gamma, \tag{9}$$

instead of boundary conditions (3)–(6). We need to remark that we really know the force f_α on the free boundary only. On other parts of the boundary we will calculate the force during the solution. Let χ_α and ψ be smooth fields in the region g related by

$$\partial_\alpha \chi_\beta + \partial_\beta \chi_\alpha = 2\psi \delta_{\alpha\beta}, \tag{10}$$

Multiplying the motion equation (1) by χ_α , integrating over g , and using (2), (9), (10), we obtain

$$\int P\psi dg = -0.5 \int f_\alpha \chi_\alpha d\gamma. \tag{11}$$

According to (10), ψ and χ_α are harmonic functions and

$$d(\chi_1 + i\chi_2) = (\psi + i\omega) dz. \tag{12}$$

where ω is a harmonic function conjugate to ψ. Let ψ_k be a complete set of harmonic functions in the region g. Using (12) we obtain the correspondent functions $\chi_{\alpha k}$.

The complete set of analytical functions w_k in the finite region g with simple connected boundary consists of functions $z^k, k = 0, 1, \ldots$. We obtain the complete set of harmonic functions ψ_k in the form $\mathrm{Re}(w_k)$, $\mathrm{Im}(w_k)$. According to (1),(2) the pressure P is a harmonic function. We present it in the form

$$P = \sum_k p_k \psi_k. \tag{13}$$

Using the expressions (11), (13) we obtain the algebraic system for coefficients p_k:

$$\sum_k \left(\int \psi_k \psi_n dg \right) p_k = -0.5 \int f_\alpha \chi_{\alpha n} d\gamma, \quad n = 0, 1, ... \tag{14}$$

The stress tensor, expressed in terms of the Airy function φ,

$$P_{\alpha\beta} = \partial^2_{\alpha\beta}\varphi - \delta_{\alpha\beta}\partial^2_{\gamma\gamma}\varphi \tag{15}$$

satisfies the equation of motion (1) identically. The Airy function satisfies the biharmonical equation

$$\Delta^2 \varphi = 0, \quad \mathbf{x} \in g. \tag{16}$$

The boundary conditions (9) take the form

$$\partial_\tau \partial_\alpha \varphi = e_{\alpha\beta} f_\beta, \quad \mathbf{x} \in \gamma, \tag{17}$$

where ∂_τ is the derivative along the tangent to the boundary. Integrating (17) from a fixed point of the boundary to current one, we obtain

$$\partial_\alpha \varphi = e_{\alpha\beta} \int\limits_{\mathbf{x}_0}^{\mathbf{x}} f_\beta d\gamma, \quad \mathbf{x} \in \gamma. \tag{18}$$

Using (15) and the expression for the Newtonian stress tensor, we obtain

$$d(\partial_\alpha \varphi) = 2\mu dV_\alpha + d\Phi_\alpha, \quad d(\Phi_1 + i\Phi_2) = P + i\Omega, \tag{19}$$

where

$$\partial_\alpha \Phi_\beta + \partial_\beta \Phi_\alpha = 2P\delta_{\alpha\beta}, \tag{20}$$

$\Omega = \mu(\partial_2 V_1 - \partial_1 V_2)$ is the harmonic function conjugate to P. Comparing (20) with (10) and using (13), we get the expression for Φ_α:

$$\Phi_\alpha = \sum_k p_k \chi_{\alpha k}. \tag{21}$$

Therefore, we obtain the expression for velocity:

$$V_\alpha = \frac{1}{2\mu}(\partial_\alpha \varphi - \Phi_\alpha), \quad \mathbf{x} \in g. \tag{22}$$

On the boundary $\partial_\alpha \varphi$ was calculated above (18). To find φ (and, respectively, the velocity V_α) in the region g, we solve the equation (16) with boundary conditions (18).

3. Calculation of the pressure and velocity with various boundary conditions

If the free boundary conditions are specified on the total boundary, then (22) gives us the solution of our problem. In a general case (22) is true too, but on the inlet, outlet and the wall the force f_α is unknown.

On the inlet we can calculate the force with the help of (3) and differentiating (22) along of boundary:

$$f_\alpha = -e_{\alpha\beta}(2\mu\partial_\tau V_\beta^{\text{in}} + \partial_\tau \Phi_\beta), \quad \mathbf{x} \in \gamma^{\text{in}}. \tag{23}$$

On the outlet we obtain the force using (4) by differentiating (22) along of boundary:

$$f_\alpha = -n_\alpha P - \tau_\alpha n_\beta \partial_\tau \Phi_\beta, \quad \mathbf{x} \in \gamma^{\text{out}}. \tag{24}$$

The slip boundary conditions (5) on the wall and (22) give us the force distribution

$$f_\alpha = -n_\alpha f_n + \tau_\alpha f_\tau, \quad \mathbf{x} \in \gamma^{\text{wall}}, \tag{25}$$

where $f_\tau = \dfrac{1+KL}{1+2KL} n_\beta \partial_\tau \Phi_\beta$, $f_n = \tau\partial_\tau \left(\Phi_\beta + \dfrac{L\tau_\beta f_\tau}{1+KL}\right)$, K is the scalar curvature of the boundary.

Expressions (23)–(25) contain $P = \sum\limits_k p_k \psi_k$ and $\Phi_\alpha = \sum\limits_k p_k \chi_{\alpha k}$. By substituting these expression into (14) we obtain the system of algebraic equations concerning coefficients p_k. After solving this system we obtain the pressure (13) and velocity distributions (22).

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