NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2014, 5 (3), P. 400–404

CRYSTALLITE MODEL FOR FLOW IN NANOTUBE CAUSED BY WALL SOLITON

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PACS 68.90.+g, 05.60.-k

Fluid flow in a nanotube, caused by a moving soliton-like perturbation of its wall, is considered. We use a crystallite model for nanotube flow. A picture of the flow is described. The formula for crystallite velocity is derived, allowing one to find fluid flux through a nanotube.

Keywords: nanotube, soliton, flow.

Received: 2 April 2014
Revised: 10 April 2014

1. Introduction

Fluid flow in nanotubes were intensively investigated in our previous studies. This was inspired by the intriguing prospects for the possible applications to nanomembrane, nanoreactor, nanoaccumulator, etc. It should be mentioned that nanotube flow obeys a set of remarkable peculiarities, distinguishing it from classical tube flow [1-6]. It poses a problem of theoretical description of such flows. Creation of new nanodevices based on nanoflows is impossible without theoretical models giving prediction of flow character. Currently, there is no general theory for nanoflow. One has only particular models, describing some specific nanoflow features. (see, e.g., [7,8]). In the present paper, we consider fluid flow in nanotube caused by mechanical waves propagating in its walls. Such flows were actively studied in recent years [9-11]. Such deformation may be caused by mechanical action on the nanotube [12]. We consider the problem in the framework of crystallite model of nanoflow, suggested in [13,14]. The model was developed theoretically [15]. The existence of ice-like clusters, resembling a solid, was observed in earlier experiments [3]. Additional confirmation for this hypothesis was given by experiments with multi-component flow through nanotubes. The authors observed structure separation predicted by the crystallite model.

2. Model description

We consider cylindrical nanotube filled by liquid. The smallness of the Reynolds number for the nanotube flow allows us to use Stokes' approximation [15]. We treat the problem in the framework of the crystallite model. Correspondingly, we assume that the nanotube contain solid-like part of the liquid concentrated near the nanotube axis. It is separated from the nanotube boundary by liquid layer (usually, one refers to this layer as the non-autonomous phase) [18]. One can note that due to thermodynamics arguments, we can conclude that both the crystallite and the non-autonomous phase layer have some equilibrium size (radius, which depends on the temperature, type of the liquid, etc. These two factors are competitive in the nanotube, leading to some correlation between their widths in particular cases.

Thus, we have the following equations for the flow of the liquid layer (non-autonomous phase) in the nanotube under the assumption of an axisymmetric character for the flow ((r, z) are the cylindrical coordinates):

$$\begin{gathered}\frac{\partial^2 v_z}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) = \frac{1}{\mu}\frac{\partial p}{\partial z},\\ \frac{\partial^2 v_r}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_r}{\partial r}\right) - \frac{1}{r^2}v_r = \frac{1}{\mu}\frac{\partial p}{\partial r},\\ \frac{\partial v_z}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(r v_r) = 0,\end{gathered} \tag{1}$$

where t is time, v_r and v_z are radial and longitudinal components of the velocity, p is the pressure, μ is the fluid viscosity. Note that the last equation is the continuity equation. We assume that the central part of the nanotube is occupied by a crystallite of radius R_c, R is the cylindrical nanotube radius. We assume that there is moving wall soliton, i.e. moving boundary perturbation. In our model, the nanotube is assumed to be cylindrical. To take into account the soliton, we pose the following non-homogeneous boundary condition at the cylinder boundary $r = R$:

$$v_z|_{r=R} = 0, \quad v_r|_{r=R} = \frac{\partial h}{\partial t} \equiv -V\frac{\partial h}{\partial z}. \tag{2}$$

Here, $h = h(z, t)$ is the radial perturbation of nanotube wall due to the soliton, V is the soliton velocity (given). As for the internal cylinder (crystallite-fluid boundary), the following boundary conditions are assumed:

$$v_z|_{r=R_c} = V_c, \quad v_r|_{r=R_c} = 0. \tag{3}$$

Here, V_c is the crystallite velocity, which is not predetermined. We consider the equilibrium state and determine the crystallite velocity using conditions of vanishing friction force (crystallite-fluid). One can present the velocity in the layer between the wall of the nanotube and the crystallite in the following form:

$$v_r = -\frac{1}{r}\frac{\partial \Psi}{\partial z}, \quad v_z = \frac{1}{r}\frac{\partial \Psi}{\partial r} + V_c\frac{\ln(R/r)}{\ln(R/R_c)}. \tag{4}$$

Substituting (4) into (1), one obtains the equation for Ψ. We present Ψ in the following form: $\Psi = \psi + \psi_0$, where ψ_0 has the form:

$$\psi_0 = \frac{V_c}{4\ln\left(\frac{R}{R_c}\right)}\left[r^2\left(1 - 2\ln\left(\frac{r}{R}\right)\right) - R_c^2\left(1 - 2\ln\left(\frac{R_c}{R}\right)\right)\right].$$

Then, the solution : ψ satisfying boundary conditions (2), (3) has the following form:

$$\psi(z, r) = \int_{-\infty}^{\infty} G(z - z', r)\, h(z')\, dz', \quad G(z, r) = \frac{V}{\pi}\int_0^{\infty} g_k(r)\cos(kz)\, dk, \tag{5}$$

where

$$\begin{gathered}g_k(r) = \frac{r(q_1 p_1 - q_2 p_2)}{\gamma(kR)\left(U_{11}(R)U_{22}(R) - U_{12}(R)U_{21}(R)\right)},\\ q_1 = \left(U_{21}(R)I_0(kR) + U_{22}(R)K_0(kR)\right),\\ p_1 = \left(U_{11}(r)I_1(kr) + U_{12}(r)K_1(kr)\right),\end{gathered}$$

$$q_2 = \left(U_{11}\left(R\right) I_0\left(kR\right) + U_{12}\left(R\right) K_0\left(kR\right)\right),$$
$$p_2 = \left(U_{21}\left(r\right) I_1\left(kr\right) + U_{22}\left(r\right) K_1\left(kr\right)\right).$$

Here,

$$U_{11}\left(r\right) = -\frac{1}{k}\int_{R_c}^{r}\frac{I_1\left(kr'\right) K_1\left(kr'\right) dr'}{\gamma\left(kr'\right)},\quad U_{12}\left(r\right) = \frac{1}{k}\int_{R_c}^{r}\frac{I_1^2\left(kr'\right) dr'}{\gamma\left(kr'\right)},$$
$$U_{21}\left(r\right) = -\frac{1}{k}\int_{R_c}^{r}\frac{K_1^2\left(kr'\right) dr'}{\gamma\left(kr'\right)},\quad U_{22}\left(r\right) = \frac{1}{k}\int_{R_c}^{r}\frac{I_1\left(kr'\right) K_1\left(kr'\right) dr'}{\gamma\left(kr'\right)},$$
$$\gamma\left(kr\right) = I_1\left(kr\right) K_0\left(kr\right) - I_0\left(kr\right) K_1\left(kr\right),$$

where $I_0\left(x\right)$, $K_0\left(x\right)$, $I_1\left(x\right)$, $K_1\left(x\right)$ are, correspondingly, the modified Bessel function and the modified Neumann function of the 0th and the 2nd orders.

Fig. 1 shows the pattern of the flow in the nanotube between the crystallite (on the left) and the nanotube wall (on the right).

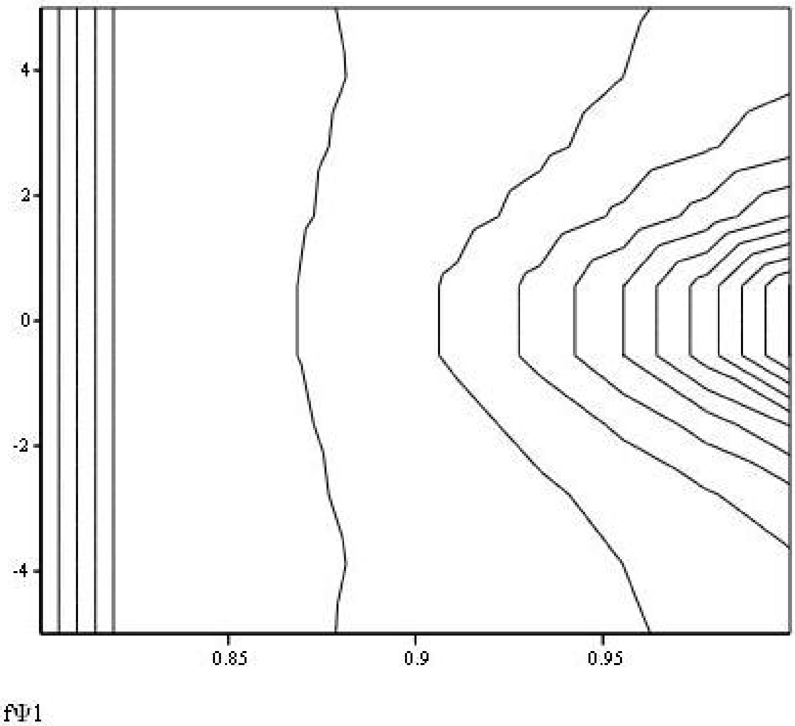

FIG. 1. Picture of the streamlines in the nanotubes

Fig. 2 shows the pattern of the flow in the nanotube. The streamlines form reflects the impact of the soliton in the right part of the figure.

Note that at present, our solution has a free parameter V_c (velocity of the crystallite). To calculate the speed of the crystallite, we use the condition of vanishing viscous friction force applied to the crystallite (more precisely, linear force density, i.e. the force, corresponding to the unit length). Then, we have:

$$V_c = \frac{2VR_c}{\pi L}\ln\left(\frac{R}{R_c}\right)\int_0^{\infty}\frac{\sin\left(kL/2\right) h_k\left(q_1 I_1\left(kR_c\right) - q_2 K_1\left(kRc\right)\right)}{k\gamma\left(kR\right)\left(U_{11}\left(R\right) U_{22}\left(R\right) - U_{12}\left(R\right) U_{21}\left(R\right)\right)}dk, \tag{6}$$

where L — crystallite length, h_k is the Fourier transform of h. Incorporating this formula with the expression for the stream function, one obtains the fluid flux through the nanotube.

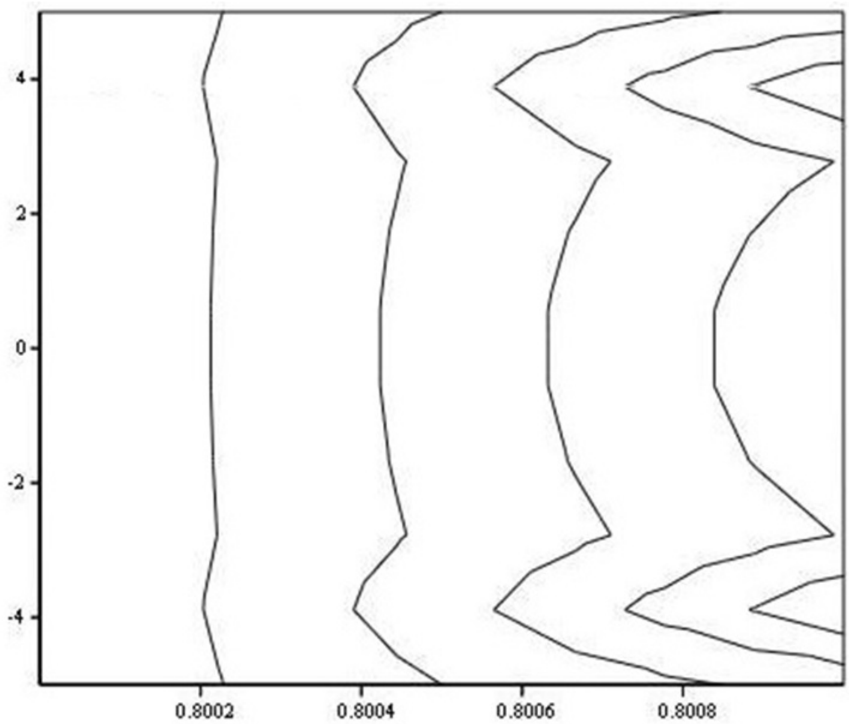

FIG. 2. Picture of the streamlines in the nanotubes

Acknowledgements

This work was partially financially supported by the Government of the Russian Federation (grant 074-U01), by the Ministry of Science and Education of the Russian Federation (GOSZADANIE 2014/190, Project 14.Z50.31.0031), by grants of the President of Russia (state contracts 14.124.13.2045-MK and 14.124.13.1493-MK).

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