On the metric graph model for flows in tubular nanostructures

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DOI 10.17586/2220-8054-2019-10-1-6-11

A metric graph model is suggested for the Stokes flow concentrated in the vicinity of a network embedded in \mathbb{R}^3 . As a basic problem, we consider the case corresponding to strong variation of the viscosity and density in a cylinder of small radius. An equation for the main term of the asymptotics is obtained. As for a graph structure, coupling conditions are assumed at the graph vertices.

Keywords: stokes flow, metric graph.

Received: 12 November 2018

Revised: 23 January 2019

1. Introduction

Many physical systems demonstrate flows concentrated near a network, e.g., flows through nanotubes [1–3] or biophysical flows [4–6]. Mentioned flow concentration near lines or surfaces may be caused by specific variation of viscosity. It is typical, for instance, for geophysical flows [7–10]. Narrowness of the domain means small ratio of width and length. It is worth noting that works concerning to viscous wires with free surface [11,12] are related to glass and fiber technologies. The problems are complicated and it is of great relevance to construct models which allow simplification.

Concentration of a solution near lines or networks appears not only in fluid mechanics but also in other fields, e.g., in quantum theory. There is an effective and simple method for investigating such systems in quantum mechanics – the quantum graph model. This method was developed in the 1980's ([13,14]) and now is a widely used approach (see, e.g., [15]). The model has some relevant features. On the one hand, it allows one to obtain explicit solutions of the model problem; in addition, it permits good approximation in many particular physical problems (see, e.g., [16–18]). This is one reason for seeking of a new field of application for such an effective instrument. In this paper, we make steps to the development of a model analogs to the quantum graph for fluid mechanics.

There are several ways to consider the hydrodynamic equations on a network (metric graph). One can deal with the 1D Navier–Stokes equation. For example, for compressible fluid of constant viscosity $\tilde{\eta}$ it takes the form:

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} - \tilde{\eta} \frac{\partial^2 v_x}{\partial x^2} = 0.$$

This is a nonlinear equation. To get the corresponding linear one we can linearize it in the vicinity of some solution or simply neglect the nonlinear inertial terms. It is possible to obtain the 1D Navier–Stokes equation by the asymptotic procedure for 3D or 2D Navier–Stokes equations in thin tubes (see, e.g., [19–22]). It is also possible to study linear 2D or 3D Stokes equations in a system of narrow tubes and to consider the limiting procedure for tubes having widths tending to zero. One observes an analogous situation for waveguides and thick quantum graphs (see, e.g., [23–25]). In the most popular model for the Stokes flow in a network one assumes that there is the Poiseuille flow in the tubes [26]). In our case the situation is more complicated (the flow is not localized inside tubes, the viscosity and the density varies essentially), and this model is not appropriate. We use the asymptotic approach. The first step was made in [27], where a metric graph model was constructed for 2D case. As a result, we obtain 1D problem on a metric graph for the main term of the asymptotic expansion. We called it the Stokes graph. In the present paper, we construct the model for 3D case.

2. Preliminaries

3D Stokes and continuity equation for the case of variable viscosity and density in cylindrical coordinates (r, φ, z) are as follows:

$$\begin{aligned} (\nabla \cdot \sigma)_r &= -\rho G_r, \\ (\nabla \cdot \sigma)_\phi &= -\rho G_\phi, \\ (\nabla \cdot \sigma)_z &= -\rho G_z, \end{aligned} \tag{1}$$

$$\nabla(\rho v) = 0. \tag{2}$$

Here σ is the stress tensor, ρ is the density, G is the external force, v is the flow velocity. In cylindrical coordinates the continuity equation (2) takes the form:

$$\frac{\rho v_r}{r} + \frac{\partial(\rho v_r)}{\partial r} + \frac{1}{r} \frac{\partial(\rho v_{\phi})}{\partial \phi} + \frac{\partial(\rho v_z)}{\partial z} = 0$$
(3)

The divergence of a total stress tensor in cylindrical coordinates have the form:

$$\begin{split} (\nabla \cdot \sigma)_r &= \frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\phi\phi}}{r} + \frac{1}{r} \frac{\partial \sigma_{\phi r}}{\partial \phi} + \frac{\partial \sigma_{zr}}{\partial z}, \\ (\nabla \cdot \sigma)_\phi &= \frac{\partial \sigma_{r\phi}}{\partial r} + \frac{2\sigma_{r\phi}}{r} + \frac{1}{r} \frac{\partial \sigma_{\phi\phi}}{\partial \phi} + \frac{\partial \sigma_{z\phi}}{\partial z}, \\ (\nabla \cdot \sigma)_z &= \frac{\partial \sigma_{rz}}{\partial r} + \frac{\sigma_{rz}}{r} + \frac{1}{r} \frac{\partial \sigma_{\phi z}}{\partial \phi} + \frac{\partial \sigma_{zz}}{\partial z}. \end{split}$$

Then equations (1) transform to the form:

$$\frac{\partial \tau_{rr}}{\partial r} + \frac{\tau_{rr} - \tau_{\phi\phi}}{r} + \frac{1}{r} \frac{\partial \tau_{r\phi}}{\partial \phi} + \frac{\partial \tau_{rz}}{\partial z} - \frac{\partial P}{\partial r} = -\rho G_r,\tag{4}$$

$$\frac{\partial \tau_{r\phi}}{\partial r} + \frac{2\tau_{r\phi}}{r} + \frac{1}{r}\frac{\partial \tau_{\phi\phi}}{\partial \phi} + \frac{\partial \tau_{\phi z}}{\partial z} - \frac{1}{r}\frac{\partial P}{\partial \phi} = -\rho G_{\phi},\tag{5}$$

$$\frac{\partial \tau_{rz}}{\partial r} + \frac{\tau_{rz}}{r} + \frac{1}{r} \frac{\partial \tau_{\phi z}}{\partial \phi} + \frac{\partial \tau_{zz}}{\partial z} - \frac{\partial P}{\partial z} = -\rho G_z.$$
(6)

In cylindrical coordinates, the deviatoric stress tensor has the following components:

$$\tau_{rr} = 2\eta \frac{\partial v_r}{\partial r}, \quad \tau_{\phi\phi} = 2\eta \left(\frac{1}{r} \frac{\partial v_{\phi}}{\partial \phi} + \frac{v_r}{r}\right), \quad \tau_{zz} = 2\eta \frac{\partial v_z}{\partial z},$$
$$\tau_{r\phi} = \eta \left(\frac{1}{r} \frac{\partial v_r}{\partial \phi} + \frac{\partial v_{\phi}}{\partial r} - \frac{v_{\phi}}{r}\right), \quad \tau_{rz} = \eta \left(\frac{\partial v_z}{\partial r} + \frac{\partial v_r}{\partial z}\right),$$
$$\tau_{\phi z} = \eta \left(\frac{\partial v_{\phi}}{\partial z} + \frac{1}{r} \frac{\partial v_z}{\partial \phi}\right).$$

In more detail, equations (4), (5), (6) take the form:

+

$$2\frac{\partial\eta}{\partial r}\frac{\partial v_r}{\partial r} + 2\eta\frac{\partial^2 v_r}{\partial r^2} + 2\eta\frac{1}{r}\frac{\partial v_r}{\partial r} - 3\eta\frac{1}{r^2}\frac{\partial v_\phi}{\partial \phi} - 2\eta\frac{v_r}{r^2} + \frac{1}{r^2}\frac{\partial\eta}{\partial \phi}\frac{\partial v_r}{\partial \phi} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_\phi}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \phi^2} + \frac{\partial^2 v_r}{\partial r^2} - \frac{\partial^2 v_r}{\partial r} - \frac{\partial^2 v_r}{\partial r^2} + \frac{\partial^$$

3. Stokes graph model

We will consider the flow under some axisymmetric conditions. Keeping in mind future replacement of variables, we change notations. Namely, we equip all variables and parameters in equations (3), (7), (8), (9) by \tilde{z} : $\tilde{r}, \tilde{\varphi}, \tilde{z}, \tilde{\eta}, \tilde{\rho}$. We will deal with the case when the values of the viscosity $\tilde{\eta}$ and the density $\tilde{\rho}$ are smooth and outside the cylinder $\{(\tilde{r}, \tilde{\varphi}, \tilde{z}) : \tilde{z} \in (-\infty, \infty), \tilde{r} \in (0, \varepsilon)\}$ are essentially greater than inside it $((\tilde{r}, \tilde{\varphi}, \tilde{z})$ are the cylindrical coordinates):

$$\begin{split} \tilde{\eta}(\tilde{r},\tilde{\varphi},\tilde{z}) &= \eta(\tilde{z})\eta_2(\tilde{r}), \quad \tilde{\rho}(\tilde{r},\tilde{\varphi},\tilde{z}) = \rho(\tilde{z})\rho_2(\tilde{r}) \\ \eta_2(\tilde{r}) &= \begin{cases} 1, & 0 \leq \tilde{r} \leq \varepsilon, \\ \eta_w, & \tilde{r} > 2\varepsilon, \end{cases} \quad \eta_w \gg 1, \\ \rho_2(\tilde{r}) &= \begin{cases} 1, & 0 \leq \tilde{r} \leq \varepsilon, \\ \rho_w, & \tilde{r} > 2\varepsilon, \end{cases} \quad \rho_w \gg 1. \end{split}$$

Here, ε is a small parameter. It means that the flow is essentially inside the cylinder. We will consider the flow inside the cylinder only. Let us introduce new coordinates: $z = \tilde{z}$, $r = \tilde{r}/\varepsilon$, $\varphi = \tilde{\varphi}$. We will consider an axisymmetric solution. Correspondingly, the flow velocity and the pressure do not depend on φ . Correspondingly, equation (8) becomes the identity. Equations (7), (9), (3) take the following form after the coordinate replacement:

$$2\varepsilon^{-2}\frac{\partial\eta}{\partial r}\frac{\partial v_r}{\partial r} + 2\varepsilon^{-2}\eta\frac{\partial^2 v_r}{\partial r^2} + 2\varepsilon^{-2}\eta\frac{1}{r}\frac{\partial v_r}{\partial r} - 2\varepsilon^{-2}\eta\frac{v_r}{r^2} + \varepsilon^{-1}\frac{\partial\eta}{\partial z}\frac{\partial v_z}{\partial r} + \varepsilon^{-1}\frac{\partial\eta}{\partial z}\frac{\partial v_r}{\partial z} + \varepsilon^{-1}\eta\frac{\partial^2 v_z}{\partial r\partial z} + \eta\frac{\partial^2 v_r}{\partial z^2} - \varepsilon^{-1}\frac{\partial P}{\partial r} = -\rho G_r,$$
(10)

$$\varepsilon^{-2} \frac{\partial \eta}{\partial r} \frac{\partial v_z}{\partial r} + \varepsilon^{-1} \frac{\partial \eta}{\partial r} \frac{\partial v_r}{\partial z} + \varepsilon^{-2} \eta \frac{\partial^2 v_z}{\partial r^2} + \varepsilon^{-1} \eta \frac{\partial^2 v_r}{\partial z \partial r} + \varepsilon^{-2} \eta \frac{1}{r} \frac{\partial v_z}{\partial r} + \varepsilon^{-1} \eta \frac{1}{r} \frac{\partial v_r}{\partial r} + 2\eta \frac{\partial^2 v_z}{\partial z^2} + 2 \frac{\partial \eta}{\partial z} \frac{\partial v_z}{\partial z} - \frac{\partial P}{\partial z} = -\rho G_z, \tag{11}$$

$$\varepsilon^{-1} \frac{\rho}{r} v_r + \varepsilon^{-1} \frac{\partial \rho}{\partial r} v_r + \varepsilon^{-1} \rho \frac{\partial v_r}{\partial r} + \frac{\partial (\rho v_z)}{\partial z} = 0.$$
(12)

We will seek the solutions in the form of series in ε :

$$v_r = v_r^0 + v_r^1 \varepsilon + \dots, \ v_z = v_z^0 + v_z^1 \varepsilon + \dots, \ P = P^0 + P^1 \varepsilon + \dots$$

Let us insert the series (3) into equations (10), (11), (12) and collect terms of the same powers of ε . We obtain the chain of equations for the series coefficients. Terms of order ε^{-2} are in the Stokes equations (in new variables) only:

$$\eta \frac{\partial^2 v_r^0}{\partial r^2} + \frac{1}{r} \frac{\partial (r\eta)}{\partial r} \frac{\partial v_r^0}{\partial r} - \frac{\eta}{r^2} v_r^0 = 0,$$
(13)

$$\eta \frac{\partial^2 v_z^0}{\partial r^2} + \frac{1}{r} \frac{\partial(r\eta)}{\partial r} \frac{\partial v_z^0}{\partial r} = 0.$$
(14)

Equation (14) gives us:

$$v_z^0(r,z) = \frac{f(z)}{\eta(z)} \int \frac{dr}{r\eta_2(r)} = u(z) \int \frac{dr}{r\eta_2(r)}.$$
(15)

Here u(z), f(z) are some functions of one variable. They should be determined later. Terms of order ε^{-1} are in three equations. The continuity equation gives us: $v_r^0 = g(z)/(r\rho)$. To avoid contradiction with (13), we conclude that $v_r^0 = 0$, i.e. the series for v_r starts from another power than for v_z . It is a conventional situation when one has different scales for different directions (see, e.g., [31]). The Stokes equations (10), (11) give us the following relations for the terms of this order:

$$\eta \frac{\partial^2 v_r^1}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} (r\eta) \frac{\partial v_r^1}{\partial r} - \frac{\eta}{r^2} v_r^1 = -\frac{\partial \eta}{\partial z} \frac{\partial v_z^0}{\partial r} - \eta \frac{\partial^2 v_z^0}{\partial r \partial z} + \frac{\partial P^0}{\partial r},$$
$$\frac{\eta}{\partial r} \frac{\partial v_z^1}{\partial r} + \eta \frac{\partial^2 v_z^1}{\partial^2 r} + \frac{1}{r} \frac{\partial v_z^1}{\partial r} = 0.$$

These equations are solvable with respect to v_r^1, v_{yz}^1 . The pressure term P^0 should be determined later.

Consider the terms of order ε^0 . The continuity equation (12) leads to the following equation for v_r^1 :

$$\frac{\partial \rho}{\partial r}v_r^1 + \frac{\rho}{r}v_r^1 + \rho\frac{\partial v_r^1}{\partial r} = -\frac{\partial \rho}{\partial z}v_z^0 - \rho\frac{\partial v_z^0}{\partial z},\tag{16}$$

Equation (10) gives the relation:

$$2\eta \frac{\partial^2 v_r^2}{\partial r^2} + 2\frac{\partial \eta}{\partial r} \frac{\partial v_r^2}{\partial r} + 2\frac{\eta}{r} \frac{\partial v_r^2}{\partial r} - 2\eta \frac{v_r^2}{r^2} = -\frac{\partial \eta}{\partial z} \frac{\partial v_z^1}{\partial r} - \frac{\partial \eta}{\partial z} \frac{\partial v_r^1}{\partial z} - \eta \frac{\partial^2 v_z^1}{\partial z \partial r} + \frac{\partial P^1}{\partial r} - \rho G_r,$$
(17)

Equation (11) produces the relation:

$$\eta \frac{\partial^2 v_z^2}{\partial r^2} + \frac{\partial \eta}{\partial r} \frac{\partial v_z^2}{\partial r} + \frac{\eta}{r} \frac{\partial v_z^2}{\partial r} = -\frac{\partial \eta}{\partial r} \frac{\partial v_z^1}{\partial z} - \frac{\partial \eta}{\partial z} \frac{\partial v_z^0}{\partial z} - \eta \frac{\partial^2 v_r^1}{\partial z \partial r} - \frac{\eta}{r} \frac{\partial v_z^1}{\partial z} - 2\eta \frac{\partial^2 v_z^0}{\partial z^2} + \frac{\partial P^0}{\partial rz} - \rho G_z.$$
(18)

The pressure is determined at the next stage (by taking into account the solvability condition $\left(\frac{\partial^2 P^0}{\partial r \partial z} = \frac{\partial P^0}{\partial z \partial r}\right)$ where the right hand side is obtained as a derivative with respect to r of the expression obtained from (18) and the left hand side – as a derivative in respect to z of the expression obtained from (17)). If we consider the first term of the asymptotic series for the velocity only, we obtain an interesting equation for v_z^0 from (18) and (16):

$$\frac{\partial^2 v_z^0}{\partial z^2} - \frac{\partial \eta}{\partial z} \frac{1}{\eta} \frac{\partial \rho}{\partial z} \frac{1}{\rho} v_z^0 = -\frac{\rho}{\eta} G_z + \frac{1}{\eta} \frac{\partial P^0}{\partial z}.$$
(19)

Taking into account the expressions for η , ρ , v_z^0 , one can see that it leads to the following equation for the function u(z) in the homogeneous case $\left(G_x = 0, \frac{\partial P^0}{\partial z} = 0\right)$:

$$u'' - \frac{\eta'}{\eta} \frac{\rho'}{\rho} u = 0.$$
⁽²⁰⁾

One can see that we have the 1D Schrödinger equation with a specific potential for the function u(x) corresponding to zero energy (the similar problem for the quantum graph is known as the threshold resonance, see, e.g., [28]).

Thus, for the flow concentrated near a line (a thin cylinder) we have one-dimensional model. Correspondingly, more complicated case of flow concentrated near a network (system of coupled segments) can be reduced to the corresponding metric graph with the Schrödinger operator:

$$H = -\frac{d^2}{dx^2} + \frac{\eta'}{\eta}\frac{\rho'}{\rho}$$

on the edges as the first approximation for the description of the flow. We call it the Stokes graph (Γ). It is necessary to determine boundary conditions at the graph vertices. Consider a vertex (let it be zero point) with *n* output edges. From physical conditions, one has:

$$\rho_1(0) = \rho_2(0) = \cdots \rho_n(0) = \rho(0)$$

and

$$u_1'(+0) = u_2'(+0) = \cdots u_n'(+0) = u'(0).$$

Here indices mark the edges $(u_j \text{ is the value of } u \text{ at } j\text{-th edge})$. The last condition is related to the pressure continuity (see, e.g., [26, 29, 30]). Here, $u_j'(+0)$ is the derivative in the outgoing direction at the vertex 0. The continuity equation gives us for this vertex:

$$\sum_{j=1}^{n} u_j = -\left(\frac{\rho(0)}{\sum_{j=1}^{n} \rho'_j(+0)}\right) u'(0).$$
(21)

It is similar to well-known δ' -coupling condition for the quantum graph [15]. The coupling constant is related to the density derivative.

We will consider the following case: $q = \frac{\eta' \rho'}{\eta \rho}$ is uniformly continuous on every edge of the graph Γ (we mark the set of its edges as E and the set of its vertices as V),

$$\theta = \frac{\rho\left(0\right)}{\sum_{j=1}^{n} \rho_{j}'\left(+0\right)}$$

is positive. We will deal with the following homogeneous equation:

$$(Hu)(x) = 0. (22)$$

Here, operator H is defined as follows. At each edge it acts as:

$$(Hu)(x) = -\frac{d^2}{dx^2}u(x) + q(x)u(x), x \in E(\Gamma).$$
(23)

Elements from its domain belong to the Sobolev space H^2 at each edge. As for vertices, the following condition takes place (for a vertex x having n output edges):

$$u_{1}'(+x) = u_{2}'(+x) = \cdots u_{n}'(+x) = u'(x), x \in V(\Gamma),$$
(24)

$$\sum_{j=1}^{\infty} u_j(x) + \theta u'(x) = 0, x \in V(\Gamma), \theta > 0.$$

$$(25)$$

$$u\left(a\right) = 0, a \in \partial\Gamma. \tag{26}$$

One can see that we have constructed a metric graph model which coincides with that of the two-dimensional case [27]. Of course, the definition of the function u differs from that of the 2D case but the model operator is the same. Correspondingly, one can obtain the same result for "cylindrical" case. Namely, we obtain the following statement.

Definition. Operator H is denoted as sign preserving on the graph Γ if the inequality u(x)u(x') > 0 takes place for any nontrivial solution of equation (22). Here x, x' are arbitrary points of $\Gamma \setminus \partial \Gamma$.

The main result of the paper is the following inequality (27) that is analogous to the Harnack's inequality for an elliptic operator on a manifold.

Main Theorem. Let H be sign preserving on graph Γ . Then there exists a constant γ , determined by the operator H and the structure of the graph Γ only, such that each non-negative on Γ solution u(x) of inequality $Hu \ge 0$ satisfies the following inequality:

$$\max_{x \in \Gamma_0} u(x) \le \gamma \min_{x \in \Gamma_0} u(x),$$
(27)

on any locally compact (in respect to Γ) subgraph $\Gamma_0, \Gamma_0 \subset \Gamma$.

Acknowledgements

This work was partially financially supported by the Government of the Russian Federation (grant 08-08), by grant 16-11-10330 of Russian Science Foundation. E. Milakis was partially supported by Research Promotion Foundation (Cyprus) grant no Excellence/1216/0025.

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