Influence of flexible particle presence on the flow in the channels of microfluidic devices. Problem statement

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Abstract. At the present paper the viscoelastic fluid flow in the element of microfluidic devices is considered. Numerical simulations were made by the FENE-P model. The element of microfluidic devices was considered as a channel with narrowing. The simulation parameters are: Reynolds number $Re = 0.01$, Weissenberg number $We = 0.6$, retardation coefficient $\beta = 0.1$ and degree of unraveling of the flexible particle $L^2 = 50, 700$.

1. Introduction
Development of micro- and nanotechnologies caused the development of such systems as "Micro Total Analysis System" or "lab-on-a-chip". These systems are characterized by the ability to carry out consistent transformations of samples (reagents). Separation, concentration, mixing of samples and moving them into micro-reaction chambers at one device made possible to obtain results in a short time. These devices are relatively new, that is why the general design guidelines or rules have not yet been developed. Organization the fluid flow through the microchannels is the basis of any device for analysis. The design of micro-devices primarily is determined by the operations that are planned to be carried out.

The aim of this paper is a mathematical problem statement of non-Newtonian viscoelastic fluid flow in a planar channel with narrowing of 50% in the laminar flow regime.

2. Governing equations
Numerical simulations were made by the FENE-P (Finitely Extensible Nonlinear Elastic by Peterlin). It applies for dilute polymer solutions and predicts the following properties: viscosity anomaly, relaxation time and dependence of longitudinal viscosity on longitudinal deformation rate. This model considers the macromolecules as flexible dumbbells (two beads connected with the spring). It assumes that the flexible dumbbells may be stretched relative to its equilibrium length [1,2,3]. Further a flexible dumbbell will be named as flexible particle.

An isothermal fluid flow is described by the momentum and mass conversation equations [2]:

\[ \rho \left( \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} \right) = -\nabla p + \vec{\tau}, \]

\[ \nabla \cdot \vec{v} = 0, \]

(1)

(2)
\[
\bar{\tau} = \bar{\tau}^p + \bar{\tau}^s, \quad \bar{\tau}^p = \eta^p \left[ \frac{\bar{\lambda}}{\lambda} - \frac{I}{1 - \frac{1}{L^2}} \right], \quad \bar{\tau}^s = 2\eta^s \bar{D}.
\]

\[
\frac{\bar{\lambda}}{1 - (\text{tr} \bar{A})/(3L^2)} + \text{We} \bar{A} = \frac{\bar{I}}{1 - 1/L^2}, \quad \bar{A} = \bar{\omega} + \bar{v} \cdot \nabla \bar{A} - \bar{A} \cdot (\bar{v} \nabla)'.
\]

where \( \bar{v} \) - velocity vector; \( \rho \) - fluid density; \( \bar{\tau} \) - stress relaxation time; \( \eta^0 = \eta^s + \eta^p \) - total viscosity; \( \eta^p \) - dynamic viscosity of non-Newtonian contribution at zero shear rate; \( \eta^s \) - dynamic viscosity of solvent contribution; \( \bar{\tau}^p \) - non-Newtonian stress contribution; \( \bar{\tau}^s \) - Newtonian stress contribution; \( \bar{\lambda} = \frac{3(\bar{Q} \bar{Q})}{Q_{eq}} \) - configuration tensor, where \( \bar{Q} \bar{Q} \) - dyadic multiplication of configuration’s tensors; \( \bar{D} = \frac{1}{2} \left( \bar{\nabla} \bar{v} + (\bar{\nabla} \bar{v})' \right) \) - strain rate tensor, where \( (\cdot)' \) - transpose procedure.

The governing equations could be written in the dimensionless form and contain the following parameters:

\[
\text{We} = \frac{\bar{\lambda} U}{l}, \quad \text{Re} = \frac{\rho Ul}{\eta^p}, \quad \beta = \frac{\eta^s}{\eta^p}, \quad L^2 = \frac{3}{\text{We}} \left( \frac{Q_{eq}}{Q_{eq}} \right)^2,
\]

where \( U \) - characteristic velocity; \( l \) - characteristic linear scale; \( Q_{eq} \) - equilibrium length of configuration vector; \( Q_{eq} \) - maximum possible length of configuration vector.

The parameters have the following values: \( \text{We} = 0.6 \), \( \text{Re} = 100 \), \( \beta = 0.1 \), \( L^2 = 50,700 \). Schematic representation of the channel and numerical grid are performed on fig.1 and fig.2.

\( H=3 \text{ mm}, \ d=6 \text{ mm}, \ h=0.5H \) means the narrowing value is 50%.

![Fig. 1 – Schematic representation of the channel](image1)

![Fig. 2 – Numerical grid](image2)

The lengths of the input and output parts of the channel are selected taking into account the conditions of velocity profile formation at the inlet and steady flow at the outlet. In the test mode, calculations were carried out on other grids (with more and less thickening). This grid was chosen as the most optimal.
The fluid is considered as incompressible viscoelastic liquid with average density \( \rho = 1000 \text{ kg/m}^3 \), dynamical viscosity at zero shear rate \( \eta_0 = 0.005 \text{ Pa} \cdot \text{s} \) and relaxation time \( \lambda = 0.0189 \text{ s} \). The following boundary and initial conditions were established:

At the inlet section \((\Gamma_1)\) the constant velocity is established:

\[
v_x = U_x = \text{const}, \quad v_y = U_y = 0.
\] (5)

The length of the input part of the channel is selected as 4 width for the formation of the steady-state velocity profile. It means that all the perturbation at the inlet section do not impact on the flow behavior at the bifurcation area.

At the output section \((\Gamma_2)\) boundary conditions are:

\[
\frac{\partial v_x}{\partial x} = 0, \quad v_y = 0
\] (6)

At the fixed walls \((\Gamma_3)\) the non-slip boundary conditions were established:

\[
v_x = 0, \quad v_y = 0
\] (7)

3. Computational Method

The governing equations (1-4) together with boundary and initial conditions were solved by means of finite volume method (FVM). The main idea is based on the dividing the computational domain into a number of non-overlapping control volumes. Each node is located within the control volume. The differential equation is integrated for each control volume. Integration procedure implements using the piecewise profiles that describe the variations of the function between the nodes. Discrete analogue of the differential equations obtained by the above mentioned procedure includes the values of the unknown function in several nodal points. One of the important properties of the finite volume method is that it has the exact integral conservation of such quantities as mass, momentum and energy over any group of control volumes and, consequently, the entire computational domain. This property manifests itself in any number of nodal points, not only in the limiting case of a very large number. Thus, even the solution on the coarse grid satisfies the exact integral balances.

This numerical procedure is realized in Open Source Field Operation and Manipulation software package developed for the numerical simulation of continuum mechanics problems (OpenFoam) [4].

In numerical simulations the process time was divided to some certain steps making not only spatial mesh but also time. To solve the problem the Euler implicit method is used. To achieve temporal accuracy and numerical stability a Courant number of less than 1 is required:

\[
C_o = \frac{\Delta t |U|}{\Delta x},
\]

where \( \Delta t \) is the time step, \( |U| \) is the magnitude of the velocity through that cell and \( \Delta x \) is the cell size in the direction of the velocity.

Convergence of numerical solution is verified by the confirmation of results obtaining on different meshes. The obtained results the modeling was made for different meshes with less quantity of nodes and different values of refinement.

4. Conclusions

This paper is devoted to mathematical formulation of the problem of elastic-viscous fluid flow in the channel of microfluidic device with a narrowing of 50%. In some cases, a real experiment is impossible or extremely problematic. Then, a possible option for obtaining the results is to conduct a numerical experiment. The reliability of the results is determined by the use of well-known and well-established mathematical models for a certain range of tasks. The rationale for the application of the FENE-P model is to represent the internal structure of an elastically viscous non-Newtonian fluid inherent in many real fluids, as well as in the predicted properties. Taking into account the special shape of the channel with the help of the selected model, it becomes possible to obtain the most complete picture of the liquid flow in the channel.
References

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