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Microchannels flow modelling with the micropolar fluid theory

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Abstract. The aim of this paper is to study the applicability of the theory of micropolar fluids to modelling and calculating flows in microchannels depending on the geometrical dimension of the flow field. First, it will be shown that if the characteristic linear dimension of the flow becomes appropriately large, the equations describing the micropolar fluid flow can be transformed into Navier-Stokes equations. Next, Poiseuille flows in a microchannel is studied in detail. In particular, the maximal cross-sectional size of the channel for which the micropolar effects of the fluid flow become important will be established. The experimentally determined values of rheological constants of the fluid have been used in calculations.

Keywords: microflows, microchannels, micropolar fluid theory, Poiseuille flow.

1. Introduction

The last decade has been characterized by a rapid growth of interest in microflows [1], mainly due to the miniaturization of flow devices used for manipulating fluids in micromachines. Microchannels belong to the most essential part of such systems. At present, the smallest, standardized, mass-produced microchannels have width $h = 0.1$ μm. It is expected that they will soon reach a dimension of $h = 0.02$ μm [2]. Successful design of microfluidic devices involving microchannels with such small dimensions requires new methods for predicting the characteristics of a flow in them.

Numerous experimental results indicate that the classical continuum approach is not applicable to describe micro- and nano- flows. If the characteristic linear dimension of the flow field is small enough, then the measured hydrodynamic data is different from that predicted by Navier-Stokes equations [1–5]. Discrepancies concern flow characteristics, such as: volume flow rate, average velocity, pressure drop and Darcy friction factor. It seems that for such flows the most reliable predictions may be obtained from calculations at the molecular level: Direct Monte Carlo simulations for gases and Molecular Dynamic simulation for liquids. However there exists an extension of Navier-Stokes approach, the micropolar fluid theory [6, 7] which augments the classical continuum fluid mechanics by incorporating the effects of microrotation of fluid molecules, and whose hydrodynamic predictions for micro-flows agree quite well with some experimental results [8–10]. Moreover, molecular dynamic simulations results show that during the Poiseuilla flow in very narrow channels the microrotation velocity (missing in the classical Navier-Stokes theory) exists and those results agree well enough with that based on the analytical solution of the micropolar fluid flow.

From that reason it seems that the micropolar fluid theory could be a useful tool in modelling microflows, but first we should establish precisely dimension of the flow field for which the micropolar modelling can be addressed to. In this paper we focus on microchannel flows. The problem arises because some experiments and theoretical estimations indicate that for microchannel flows of real fluids the micropolar effects become important when the width of the channel is comparable to the dimensions of the fluid molecules. In such a case, it can be expected that the assumption of continuum medium model is no longer justified and flows should be modelled on the molecular level. On the other hand, when the geometrical dimensions of the flow become sufficiently large, the experimental results agree well with the Navier-Stokes hydrodynamic predictions.

Since, so far, there are no experimental methods that would allow one to measure the velocity profile and microrotation in narrow channels with diameter equal to the size of just a few molecules, the only available method to establish the validity of the micropolar model of a fluid treated as a continuous medium is to compare the results of the computer simulation based on molecular modeling with that based on the analytical solution of micropolar fluid flow. In [11–15] results of a computer simulation of plane Poiseuille flow by the Molecular Dynamics method are presented and compared with analytical solutions. These comparisons shows that the analytical solutions of the Poiseuille flow for channel widths not smaller than 10 diameters of the molecule are in a reasonable agreement with the results of the MD simulation. For narrower channels the agreement is poor.

Finding answer to the question: what is the limiting value of diameter of the microchannel below which the micropolar effects of the fluid flow are important and can not be neglected is the goal of this paper. For such or narrower channel the micropolar modelling for Poiseuille flows is more reliable than by use classical Navier-Stokes dynamics.

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2. Equations of micropolar fluid flow

Eringen formulated the micropolar fluid theory in 1966 [6] as an extension of the Navier-Stokes model of classical hydrodynamics to facilitate the description of the fluids with complex molecules. The micropolar fluids are usually defined as isotropic, polar fluids in which deformation of molecules is neglected. Physically, a micropolar model can represent fluids whose molecules can rotate independently of the fluid stream flow and its local vorticity. In other words, micropolar fluids are the medium whose behaviour during their flows is affected by the microrotation, i.e. the local rotational motion of fluid molecules contained in a given fluid volume element. The occurrence of the microrotation vector, which differs from the stream flow vorticity vector $\omega \neq \operatorname{rot} V$ and from the angular velocity $\omega \neq \frac{1}{2}\operatorname{rot} V$, results in the formation of antisymmetric stresses and coupled stresses, which consequently result in an increase in the energy dissipation. In the equations describing the flow field, there occur two independent kinematic variables: the velocity V and the microrotation ω. The vector equation, representing the conservation law of angular momentum, is added to the classical fluid dynamics equations.

The constitutive equations for micropolar fluid [6] define the stress tensor $T = \{T_{ij}\}$ which is a nonsymmetric tensor and the couple stress tensor $C = \{C_{ij}\}$ as follows:

$$T_{ij} = (-p + \lambda V_{k,k})\delta_{ij} + \mu(V_{i,j} + V_{j,i}) + \kappa(V_{j,i} - \varepsilon_{ijk}\omega_k) \tag{1}$$

$$C_{ij} = \alpha\omega_{k,k}\delta_{ij} + \beta\omega_{i,j} + \gamma\omega_{j,i} \tag{2}$$

where the symbols denote: p – pressure, λ, μ, κ – coefficients of bulk, shear and vortex viscosities, α, β, γ – the respective coefficients of coupled viscosities, ε_{ijk} – the Levi-Civita tensor, δ_{ik} – the Kronecker delta.

Here, the coefficients satisfy inequalities:

$$\kappa > 0,\ 3\lambda + \kappa + 2\mu > 0,\ 2\mu + \kappa > 0$$
$$3\alpha + 2\gamma > 0,\ -\gamma < \beta < \gamma,\ \gamma > 0.$$

An alternative form to (1) is [6]:

$$T_{ij} = (-p + \lambda V_{k,k})\delta_{ij} + (\mu + \kappa/2)(V_{i,j} + V_{j,i}) + \kappa(V_{j,i} - V_{i,j}) - \kappa\varepsilon_{ijk}\omega_k \tag{3}$$

and the symmetric part of the stress tensor T in (3) is:

$$T_{ij}^{[S]} = (-p + \lambda V_{k,k})\delta_{ij} + (\mu + \kappa/2)(V_{i,j} + V_{j,i}). \tag{4}$$

This form is just the same as the definition of the stress tensor of classical hydrodynamics, where $\mu_N = \mu + \kappa/2$ denotes the dynamic Newtonian viscosity coefficient.

If we assume that the specific internal energy of the fluid is proportional to its temperature and that Fourier law holds, then, for the flow of a micropolar incompressible fluid with constant material coefficients, the flow equations can be uncoupled from the energy conservation equation [6, 7, 16] and becomes:

$$\operatorname{div} V = 0 \tag{5}$$

$$\rho\frac{\mathrm{d}V}{\mathrm{d}t} = \rho\mathbf{f} - \operatorname{grad} p - (\mu + \kappa)\operatorname{rotrot} V + \kappa \operatorname{rot}\omega \tag{6}$$

$$\rho I\frac{\mathrm{d}\omega}{\mathrm{d}t} = (\alpha + \beta + \gamma)\operatorname{grad}\ \operatorname{div}\omega - \gamma\operatorname{rotrot}\omega + \kappa \operatorname{rot} V - 2\kappa\omega + \rho\mathbf{g} \tag{7}$$

where: ρ – fluid density
ω – microrotation, $\omega = (\omega_1, \omega_2, \omega_3)$
V – velocity, $V = (V_1, V_2, V_3)$
$\mathbf{f}$ – body force per unit mass, $\mathbf{f} = (f_1, f_2, f_3)$
$\mathbf{g}$ – body torque per unit mass, $\mathbf{g} = (g_1, g_2, g_3)$.

3. Dimensional analysis of the micropolar fluid flow equations

Our main purpose in this section is to show that if the characteristic geometrical linear dimension of the fluid flow field becomes appropriately large, the equations describing the micropolar fluid flows can be transformed into Navier-Stokes equations. We shall confine ourselves to studying a particular form of equations (6)–(7) describing micropolar fluid flows for which the body torque $\mathbf{g} = \mathbf{0}$, and the force $\mathbf{f} = \mathbf{0}$. We shall present their nondimensional form and investigate the effect of the new nondimensional microstructure parameters, following from a micropolar fluid model, on the form of the flow equations.

Let us assume that, for a particular flow relevant to the physical problem to be studied, characteristic – or reference – quantities of: linear dimension, time, velocity and density are the quantities denoted with L_c, T_c, U and p, respectively. Symbols with a prime are used to denote nondimensional quantities:

$$V' = V/U, \quad t' = t/T_c, \quad \nabla' = L_c\nabla,$$
$$\omega' = \omega L_c/U, \quad x' = x/L_c, \quad p' = \frac{p}{\frac{(\mu+\kappa)U}{L_c}} \tag{8}$$

Applying the standard method of dimensional analysis to the fluid flow equations (6)–(7) we can write them in the nondimensional form:

$$\mathrm{Re}\left(\frac{1}{\mathrm{St}}\frac{\partial V'}{\partial t'} + V'\nabla' V'\right) = -\nabla' p' - \nabla' \times \nabla' \times V' + 2N^2\nabla' \times \omega' \tag{9}$$

$$\mathrm{Re}\,\frac{I}{l^2}\left(\frac{1}{\mathrm{St}}\frac{\partial \omega'}{\partial t'} + V'\nabla'\omega'\right) = 2L^2N^2(-2\omega' + \nabla' \times V') + 2(1 - N^2)\left(\frac{\alpha + \beta + \gamma}{\gamma}\nabla'\nabla'\omega' - \nabla' \times \nabla' \times \omega'\right) \tag{10}$$

In the equations, besides classical counterparts of the nondimensional numbers: Re – Reynolds and St-Strouhal:

$$\mathrm{Re} = \frac{UL_c\rho}{\mu + \kappa} \qquad \mathrm{St} = \frac{UT_c}{L_c} \tag{11}$$

there occur new nondimensional parameters N and L:

$$N = \sqrt{\frac{\kappa}{2\mu_N + \kappa}}, \quad L = \frac{L_c}{l}, \quad l = \sqrt{\frac{\gamma}{4\mu_N}} \tag{12}$$

Parameter L, $L > 0$ characterizes the relationship between the geometric dimension of the flow L_c and the rheologic properties of fluid and is also called measure of

the relative length of the fluid microstructure. The value of l reflects the microscopic properties of the fluid [7, 16, 17] (the bigger the molecules the greater the value of the parameter l). Parameter N, $0 \leqslant N \leqslant 1$ characterizes coupling between the vortex viscosity coefficient κ and the shear viscosity coefficient μ. Let us observe that the value of the parameter N for a given fluid is constant, whereas the value of the parameter L depends explicitly on the characteristic linear dimension of the flow.

We shall now investigate what is the effect of the boundary values of these parameters on the form of the flow equations (9)–(10).

If the value of the parameter $N \to 0$, then the equations of momentum (9) and angular momentum (10) become independent of each other and the first one transforms into a classical Navier-Stokes equation for Newtonian fluid.

It is in agreement with the result obtained in paper [18] in which, in aspect of long time behavior micropolar fluid flows, it was shown that when $\kappa \to 0$ the velocity field of the micropolar fluid model converges to the velocity field of the classical Navier-Stokes model.

If the value of the parameter $L \to 0$, then the stream velocity rotation $\Delta' \times V'$ is removed from the right side of equation (10). This situation can be interpreted as a description of a fluid flow whose angular acceleration is not affected by the fluid stream vorticity. In the other limiting case, for $L \to \infty$, from the angular momentum equation (10), we obtain the relationship defining the microrotation vector as equal to one half of the vector of the fluid stream vorticity:

$$2\omega' = \nabla' \times V' \tag{13}$$

that is to say, to the angular velocity of the fluid volume element if the element moved as a rigid body. Formula (13) allows eliminating the microrotation vector from the angular momentum equation (9), which now, in dimensional variables, takes the form:

$$\rho \frac{\mathrm{d}V}{\mathrm{d}t} = -\nabla p - \mu_N \nabla \times \nabla \times V \tag{14}$$

This is the Navier-Stokes equation for Newtonian fluids.

The way we obtained this asymptotic form of micropolar fluid flow equations unmistakably indicates that the micropolar effects in the fluid flow description can be neglected only if the value of L, that is, the characteristic linear dimension of flow L_c, is sufficiently large, as $l = \text{const}$ for a given fluid. Therefore, together with a decrease in the value of L_c there will appear discrepancies between the solutions obtained through application of the micropolar and the classical fluid models.

The above result gives an answer to the fundamental question that appeared during the microflow research: why the results obtained using the classical hydrodynamics equations, with regard to the flows of the same real fluid, are in agreement with the experiment on one occasion and disagree with it on another. Besides, it indicates that for every micropolar fluid flow, if its linear dimension L_c is sufficiently large, it pays off to carry on the calculations on the basis of the classical dynamics, Navier-Stokes equations, which are simpler than those of micropolar fluid dynamic equations.

An analysis of the effect of nondimensional parameters on the form of the equations also indicates to what domain a micropolar fluid theory is suitable to be applied: to flows which occur in microdevices, defectoscopy, tribology and living organisms.

4. Analysis of Poiseuille flow modelling in microchannels

Our aim now is to predict the value of the characteristic linear dimension L_c of the microchannel flow below which the micropolar effects of the fluid during the flow appear and thus the micropolar modelling for Poiseuille flows is more reliable than when using classical Navier-Stokes dynamics. It will be done by the comparison of the volume flow rate calculations based on exact stationary solutions of the micropolar fluid and the Navier-Stokes equations of the Poiseuille flow in circular microchannels. The comparison will be performed for real fluids and in terms of dimensionless microstructural parameters. For the flows in circular microchannels the linear dimension L_c is defined as: $L_c = d$, d-diameter of the pipe.

Analytical solution of the equation describing the Poiseuille flows of micropolar fluid in the circular channel of radius R, in a cylindrical coordinates system (r, θ, z) is given by the formulae [19]:

$$\frac{V_z(\tilde{r})}{V_0} = 1 - \tilde{r}^2 + \frac{2\delta}{2+\delta} \frac{I_0(kR)}{kRI_1(kR)} \left[\frac{I_0(kR\tilde{r})}{I_0(kR)} - 1 \right] \tag{15}$$

$$\frac{\omega(\tilde{r})R}{V_0} = \tilde{r} - \frac{(2\xi+\delta)}{2+\delta} \frac{I_1(kR\tilde{r})}{I_1(kR)} \tag{16}$$

where: $V = (0, 0, V_z(r))$ – velocity vector, $\omega = (0, \omega(r), 0)$ – microrotation vector and α_0 – constant describing the fluid-wall interaction which appears in the equation defining boundary conditions for microrotation on the walls, $0 \leqslant \alpha_0 \leqslant 1$ [10, 16, 19], $p = p(z)$ pressure I_0, I_1 – are Bessel functions of first kind. The remaining symbols denote:

$$\delta = \frac{\kappa(1-\alpha_0)}{\mu_{\mathrm{N}}}, \quad k = \sqrt{\frac{(2\mu+\kappa)\kappa}{(\mu+\kappa)\gamma}} \tag{17}$$

$$\xi = 1 - \alpha_0, \quad V_0 = \frac{R^2(-dp/dz)}{4\mu_{\mathrm{N}}}, \quad \tilde{r} = \frac{r}{R} \tag{18}$$

Integrating velocity (15) over the cross section of the channel we obtain the formulae for the volume flow rate which depends on parameters δ, k and R:

$$Q_m(R) = Q_{\mathrm{N}}(R) \left\{ 1 + \frac{2\delta}{2+\delta} \frac{4}{(kR)^2} \left[1 - \frac{kRI_0(kR)}{2I_1(kR)} \right] \right\} \tag{19}$$

where $Q_N(R)$ denotes the volume flow rate of the classical, Newtonian fluid with viscosity μ_N which flows through

the microchannel of radius R and stands:

$$Q_{\mathrm{N}}(R) = \frac{\pi R^4(-dp/dz)}{8\mu_{\mathrm{N}}} \tag{20}$$

The values of the parameters δ and k can be determined experimentally [10, 19, 20]. For instance, Table 1 gives the values of the parameters for exemplifying fluids determined for the fluid flows in quartz channels [10]. The chemical composition of the fluids was given in detail in [19, 20].

To make visible the usability of micropolar fluid flow model to the flow calculations in term of the microchannel radius R, we define the relative volume flow rate $Q(R)$ – "comparison parmeter" – as a quotient:

$$Q(R) = Q_m(R)/Q_N(R) \tag{21}$$

If the value of the relative volume flow rate $Q(R) = 1$, it means that values of volume flow rate calculated by use Navier-Stokes equation and micropolar fluid dynamic equations are the same. In such situation the flow in the microchannel of radius R is well described by the classical model of the fluid, and it pays off to carry on the calculations on the basis of the classical dynamics, Navier-Stokes equations, which are simpler than those of micropolar fluid dynamic.

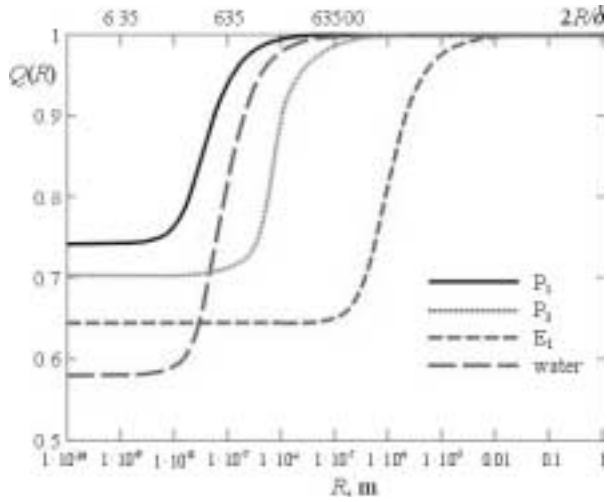

Fig. 1. Relative volume flow rate $Q(R)$ for water, fluids P_1, P_2, E_1, δ – linear dimension of water molecule, $\delta = 3.15 * 10^{-10}$ m. [21]

Table 1
Values of parameters δ, and k of some fluids, (notation after Ref. 10)

fluids	$k \cdot 10^{-7}$, m^{-1}	δ
P_1	15.20	0.695
P_2	8.75	0.800
water	7.03	1.45
E_1	5470.00	1.356

For some real fluids the curves illustrating the dependence of the relative fluid flow rate $Q(R)$ on radius R of the channel are plotted in Fig. 1. Experimental data from Table 1 were used for the calculations. Results from Fig. 1 show that, for every fluid beginning from a given channel diameter, $d = 2R$, the volume flow rate calculated using the micropolar fluid model is smaller than that calculated with the use of the classical Newtonian model of the fluid. The difference does increase with the decrease in the channel diameter. What is more important, it can be observed that for every fluid there exists its "own" limiting channel diameter from which Q values begin to decrease. The above suggests that the channel diameter size starting from which it is worthwhile to carry flow calculations based on the classical fluid model depends on fluid rheological properties – the values of viscosity coefficients.

The calculation of $Q(R)$ performed for a real fluid matches the result obtained in the previous section. The formulae describing the interrelations between the parameter groups δ and k and the parameters l and N , discussed in the previous section are as follows:

$$l^2 = \frac{\delta}{(2\xi + \delta)k^2} \tag{22}$$

$$N^2 = \frac{\delta}{(2\xi + \delta)} \tag{23}$$

where $\xi = 1 - \alpha_0$.

Table 2
Values of parameters l, and N of some fluids

Fluid	l, m.		N	
	$\alpha_0 = 0$	$\alpha_0 = 0.9$	$\alpha_0 = 0$	$\alpha_0 = 0.9$
P_1	$3.34095 \cdot 10^{-9}$	$5.79745 \cdot 10^{-9}$	0.50782	0.88921
P_2	$6.1088 \cdot 10^{-9}$	$1.022 \cdot 10^{-8}$	0.53432	0.89443
water	$9.2614 \cdot 10^{-9}$	$1.3392 \cdot 10^{-8}$	0.6483	0.93744
E_1	$1.2713 \cdot 10^{-5}$	$1.867 \cdot 10^{-5}$	0.63565	0.93352

Making use of above formulae (22) and (23) it is possible to calculate the range of the changes of l, and N values with regard to α_0 for the fluids from Table 1. The calculated values are listed in Table 2. Considering the l values given in Table 2 and results depicted in Fig. 1, it can be concluded that the greatest differences between the two fluid models occur when the value of the parameter $L = d/l$ satisfies the inequality $L < 10$. However, one can also observe that $Q(R) = 1$ if the value of parameter L satisfies the inequality $L > 1000$.

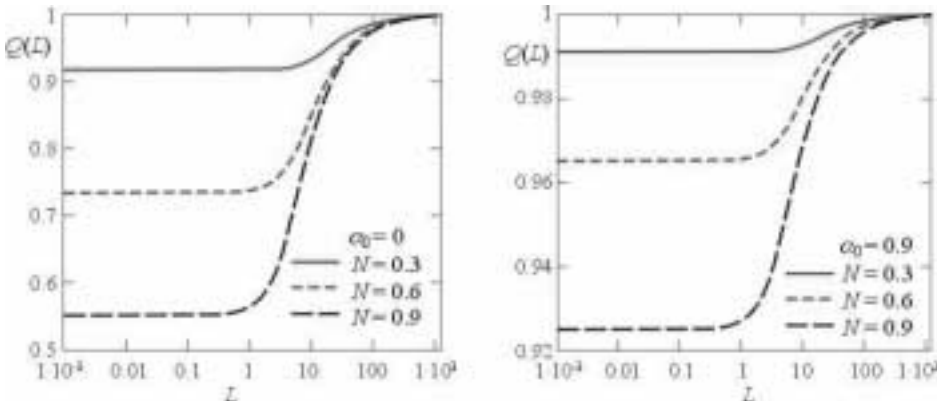

Fig. 2. Relative volume fluid flow in circular channel as a function of parameters L and N for $\alpha_0 = 0$ i 0.9

Let us now examine the effect of the microstructural parameters L and N on the relative volume flow rate in detail. Using formula (23) and (22) to (19) and (21) we obtain:

$$Q(L,N,\zeta) = \left\{1 + \frac{8N^2 2\zeta}{(2+2N^2\zeta)(LN)^2}\left[1 - \frac{LNI_0(LN)}{2I_1(LN)}\right]\right\} \quad (24)$$

Results of calculations of relative volume fluid flow rate $Q(L,N,\alpha_0)$ are depicted in Fig. 2.4. It can be observed that the Q value is strongly affected by the parameters N and α_0. An increase in the value of parameter N (at constant L and α_0 values) brings about a decrease in the value of Q. Next, an increase in the value of parameter α_0 (at constant L and N) increases the Q value. Analysing the results it can be concluded that for $L > 1000$ the value of $Q = 1$, otherwise $Q < 1$, which means that there occur discrepancies in calculations obtained making use of the two fluid models. For $L = 0$ (1) and smaller values, $Q(L,N,\alpha_0)$ value is the smallest. Obtained results match the estimates for real fluids.

To summarise the results obtained in this section we can state that the channel diameter at which micropolar effects are small enough to justify carrying out calculations based on the classical fluid dynamics crucially depends on the rheological parameters of the fluid and parameter α_0. An effective application of the micropolar fluid model for calculations depends of on the values of parameters L, N and α_0. For $L = 0$ (1), there occur maximum differences between the results of the calculations based on the two models. For $L > 1000$ there are hardly any differences.

It should be pointed out that the analysis of an effective application of a micropolar fluid theory to modeling other microflows (between squeezing plates, between converging spheres) shows exactly the same dependence of the geometrical range of its applicability on microstructure parameters L, N [21] as presented here, for flow in microchannels.

5. Concluding remarks

The analysis presented in the paper shows that the geometric size of flow field plays a crucial role in the useful applicability micropolar fluid theory to modelling microflows.

The general result was established theoretically, which shows that when the characteristic linear dimension of the flow field is large enough, the micropolar model can be reduced to the classical Navier-Stokes equation. This result was obtained through an application of dimensional analysis to the set of equations describing the micropolar fluid flow. It should be pointed out that reasoning of that type can sometimes lead to an error. This is not the case here since the classical model is not a singular perturbation of the micropolar model.

For flow in microchannels the upper limit of usability of micropolar fluid theory have been established as a result of comparing volume flow rate of Poiseuille flow based on the classical and the micropolar fluid mechanics. The experimentally determined values of rheological constants of the fluid have been used in calculations.

It was confirmed that the micropolar model is applicable for small characteristic geometrical dimension of the flow (i.e. diameter for circular channel flow). Furthermore, the particular value of the diameter of the channel for which the flow should be modelled using the micropolar approach was established. Results indicate that this "limiting dimension" depends on the rheological properties of the fluid that can be expressed through defined here nondimensional microstructure parameters.

For wider microchannels, the flow is quiet well described by the classical model of the fluid, and it pays off to carry on the calculations on the basis of the classical dynamics, Navier-Stokes equations, which are simpler than those of micropolar fluid dynamic equations.

The obtained results match some of the earlier obtained experimental estimates.

The lower limit of applicability of the micropolar fluid theory to modelling microflows as was mentioned before results from fundamental questions for how small dimensions of the flow field the micropolar fluid model

can be treated as continuum medium. This problem was investigated in other papers in detail [15, 21–23]. Based on the results it may be concluded that the micropolar theory is applicable to modelling fluid flows in channels of width not smaller than 10 diameters of the fluid molecule.

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