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Enhancement Transport Phenomena in the Navier-Stokes Shell-like Slip Layer

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Abstract: In the paper we propose to remove the classical Navier slip condition and replace it with new generalized Navier-Stokes slip boundary conditions. These conditions are postulated to be ones following from the mass and momentum balance within a thin, shell-like moving boundary layer. Owing to this, the problem consistency between the internal and external friction in a viscous fluid is solved within the framework of a proper form of the layer balances, and a proper form of constitutive relations for appropriate friction forces. Finally, the common features of the Navier, Stokes, Maxwell and Reynolds concepts of a boundary slip layer are compared and revalorized. Classifications of different mobility mechanisms, important for flows in micro- and nano-channels are discussed.

Keywords: Microflows, enhancement, velocity-slip.

1 Introduction

In the past two decades, a considerably large interest has been devoted to the new, small scale devices. Current possibilities allow manufacturing devices of order of nanometres. However, despite the capabilities in producing small scaled objects, there is an apparent lack of knowledge in their behaviour. A great example is the MEMS and NEMS [Gad-el-Hak (1991); Karniadakis, Beskok, and Aluru (2005)] class of devices. The incorporated flow phenomena there occurring are not well described. As recent study has shown the measured mass flow rate in the microscaled and nanoscaled devices is considerably larger than predicted by means of a standard fluid dynamics formulations for Poiseuille flow [Poiseuille (1846)]. This discrepancy is mostly identified to come from the velocity slip at the fluid-solid interface. The simpliest experimental setups (although exploiting most sophisticated methods) have been developed [Ewart, Perrier, Graur, and Meolans (2006); Arkilic, Schmidt, and Breuer (1997); Pitakarnnop, Varoutis, Valougeorgis, Geof-

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froy, Baldas, and Colin (2010)] to address measurement of only the velocity slip phenomenon, but also more complex investigations were carried out, where transition from laminar to turbulent flow were looked upon [Blonski (2009); Sharp and Adrian (2004)] as well as thermal [Jebauer and Czerwinska (2007); Lewandowski, Ochrymiuk, and Czerwinska (2011)] and concentration [Xu and Ju (2005); Badur, Karcz, and Lemanski (2011); Jozwik, Karcz, and Badur (2011)] jump phenomena.

Despite the achieved fluency in experimental design, there is an apparent lack of understanding of the flow enhancement in it's theoretical background. This is manifested throughout the prediction discrepancies compared to measurement. The discrepancies growth is directly proportional to the medium rarefaction, and inversely proportional to the channel hydraulic diametre. This rule also stands for other phenomena, when their influence on the bulk flow is not negligible. By the last statement it is understood, that although the phenomena may be present in a large scaled devcies, they seem to be of insignificant importance there. When the boundary layer extends to the bulk however, as it occurrs in the micro- and nanochannels, the wall effects alter the entire flow field. Recent developement in theoretical understanding of how the enhancement may work, led researchers [Deissler (1964); Colin, Lalonde, and Caen (2004); Maurer, Tabeling, Joseph, and Willaime (2003)] to the formulation of the so called "second-order" slip boundary. The idea relies on the Maxwell [Maxwell (1879)] model derived from gas kinetic theory. The veolcity derivative present in the model is perceived as the first term in the Taylor series, and hence the second order derivative is added up to the boundary condition. However correct or not this is, there is but a single flaw in the rationale. The applied second order term remains inconsistent with the definition of the stress tensor. This brings about questions to how the model may be physically interpreted, and how to regain the consistency with the continuum mechanical approach framework.

Different approaches have been proposed for modeling of the rarefied medium flow. Among them are the statistical methods (DSMC) [Aktas, Aluru, and Ravaioli (2001); Stefanov, Barber, Ota, and Emerson (2005)], (LBM) [Chen, Doolen, Eggert, and Grunau (1991); Qian, d'Humieres, and Lallemand (1992); Bhatnagar, Gross, and Krook (1954)] and explicit molecular methods (MD) [Bird (1994)]. Vast computational resources are required for the mentioned methods to be realised, and restricts the use for purely academic research with relatively simple geometrical setups. The search for universal and reliable computational tool is still under way and, unfortulately, far from being established. The need for such a model, capable of giving relatively quick results and reliable in sense of it's agreement with experimental data motivated the work at Polish Academy of Sciences Fluid Flow Machinery Institute (FFMI PASci). The model FFMI elaborates on provides an extention to the flow enhancement by means of additional to velocity slip phenomena.

The goal is then to acquire mathematical formulation for the boundary condition to be consistent with the continuum mechanics framework. The results achieved so far are shown in the paper.

2 Enhanced transport model

2.1 Boundary condition formulation

The initian point in the FFMI PASci model developement is, contrary to the commonly used and widely elaborated on Maxwell model, the boundary condition firstly introduced in 1827 by Navier in form [Navier (1827)]:

$$\nu\vec{\mathrm{v}} + \mu \frac{d\vec{\mathrm{v}}}{dn} = 0. \tag{1}$$

Further extension to the model, to the more general form was given by Cauchy, one year after Navier's paper, where physical interpretation is given to the terms in the equation [Cauchy (1828)]:

$$\vec{f} + \vec{\tau}_w = 0. \tag{2}$$

In the above Cauchy definition, $\vec{f}$ is the boundary friction force, while $\vec{\tau}_w$ is identified as the fluid "wall stress". It is a very neat representation, and to some extent complete. If one considers a simple flow of a fluid in contact with the solid wall. However, in a more general case, as Poisson has shown in his 1831 paper, the condition requires further extension for the inclusion of capillary forces, most important in case of multiphase flows. The capillary forces may have a strong influence on friction and velocity slip. The Cauchy boundary condition is hence supplemented with an additional term by Poisson, and has a form [Poisson (1831)]:

$$\vec{f} + \vec{\tau}_w + \mathrm{div}_s(\gamma \overset{\leftrightarrow}{I}_s) = 0, \tag{3}$$

where $\gamma \overset{\leftrightarrow}{I}_s$ is introduced as the capillary stress tensor. The tensor, in the framework suggested by FFMI PASci may be written as a sum:

$$\overset{\leftrightarrow}{p_s} = \overset{\leftrightarrow}{p_s}^{(v)} + \overset{\leftrightarrow}{p_s}^{(c)}, \tag{4}$$

where $\overset{\leftrightarrow}{p_s}^{(v)}$ is the conservation, elastic stresses, while $\overset{\leftrightarrow}{p_s}^{(c)}$ describe the dissipative, non-elastic stresses. Each of the stresses are defined as follows:

$$\overset{\leftrightarrow}{p_s}^{(c)} = \overset{\leftrightarrow}{\gamma}_0 \overset{\leftrightarrow}{II}_s \overset{\leftrightarrow}{\gamma}_1 + \vec{n} \otimes \overset{\leftrightarrow}{I}_s \ \mathrm{div}_s(\overset{\leftrightarrow}{\gamma}_1 - \overset{\leftrightarrow}{II}_s \overset{\leftrightarrow}{\gamma}_2); \tag{5}$$

$$\overset{\leftrightarrow}{\gamma}_0 = \gamma \overset{\leftrightarrow}{I}_s;$$

$\overleftrightarrow{\gamma}_1 = C\,\overleftrightarrow{II}_s;$

$\overleftrightarrow{\gamma}_2 = K\,\overleftrightarrow{III}_s;$

$$\overleftrightarrow{p}_s^{(v)} = \lambda'(\mathrm{tr}\,\overleftrightarrow{d}_s)\,\overleftrightarrow{I}_s + \lambda\, v_{n,n}\vec{n}\otimes\vec{n} + 2\mu'\,\overleftrightarrow{I}_s I_d\,\overleftrightarrow{I}_s + 2\mu(\overleftrightarrow{d}_s - \overleftrightarrow{I}_s I_d\,\overleftrightarrow{I}_s) \tag{6}$$

In 1845 Stokes has further expanded the boundary condition definition applying the so called wall pressure tensor. This relies on the observation that the pressure in the vicinity of the wall does not necessarily equal the pressure at the wall, which influences the overall behaviour of the fluid at the fluid-solid interface. Following Stokes, we put the boundary condition as such [Stokes (1845)]:

$$\vec{f} + \overleftrightarrow{p}\,\vec{n} + \mathrm{div}_s(\gamma\,\overleftrightarrow{I}_s) + \varpi\vec{n} = 0, \tag{7}$$

where pressure tensor $\overleftrightarrow{p}$ is defined in the following section. Given the formulations and definitions introduced so far, the generalized form of the boundary condition, as proposed by FFMI PASci team states:

$$\begin{aligned}\partial_t(\rho_s\vec{\mathrm{v}}_s) + \mathrm{div}_s(\rho_s\vec{\mathrm{v}}_s\otimes\vec{\mathrm{v}}_{s||}) - w_n I_b\rho_s\vec{\mathrm{v}}_s + \mathrm{div}_s(\overleftrightarrow{p}_s) +\\ + \frac{\partial}{\partial n}(\overleftrightarrow{p}_s\,\vec{n}) + [\overleftrightarrow{p}_A\,\vec{n}_A + \overleftrightarrow{p}_B\,\vec{n}_B + \vec{f}_{SA} + \vec{f}_{SB}] =\\ = \rho_s\vec{b}_s + \dot{m}_A(\vec{\mathrm{v}}_A - \vec{\mathrm{v}}_s) + \dot{m}_B(\vec{\mathrm{v}}_B - \vec{\mathrm{v}}_s),\end{aligned} \tag{8}$$

The above equation may be written in it's simplified form, correct for the flow of a rarefied gas in contact with a solid, inelastic wall. The boundary condition would then be of a form:

$$\begin{aligned}\partial_t(\rho_s\vec{\mathrm{v}}_s) + \mathrm{div}_s(\rho_s\vec{\mathrm{v}}_s\otimes\vec{\mathrm{v}}_{s||}) - w_n I_b\rho_s\vec{\mathrm{v}}_s + \mathrm{div}_s(\overleftrightarrow{p}_s) +\\ + \frac{\partial}{\partial n}(\overleftrightarrow{p}_s\,\vec{n}) + [\overleftrightarrow{p}\,\vec{n} + \vec{f}] = \rho_s\vec{b}_s + \dot{m}_{fluid}(\vec{\mathrm{v}} - \vec{\mathrm{v}}_s).\end{aligned} \tag{9}$$

At this point, the general formulation of the boundary condition has been given with no further explanation for the terms there appearing. The next section is devoted to defining both the friction force and the wall stress force, and also explain the pressure tensor.

2.2 Definition of friction and wall stress terms

In 1902 Duhem [Duhem (1901)] and in 1927 Roy [Roy (1927)] have been working on the velocity slip boundary condition. They assumed, that the wall friction force is determined by the definition first given by Coulomb in 1801 [de Coulomb (1801)]:

$$\vec{f} = \left(\nu\frac{1}{|\vec{\mathrm{v}}_s|} + \nu_1 + \nu_2|\vec{\mathrm{v}}_s|\right)\vec{\mathrm{v}}_s. \tag{10}$$

On the other hand, in the boundary condition definition, there exists the wall stress vector which is, in accordance to Cauchy definition, defined to be [Cauchy (1828)]:

$$\vec{\tau}_w = \overset{\leftrightarrow}{t}\ \vec{n}, \tag{11}$$

where $\overset{\leftrightarrow}{t}$ is the Cauchy tensor. In the simpliest form, the Cauchy tensor may be defined to be:

$$\overset{\leftrightarrow}{t} = -p\,\overset{\leftrightarrow}{I} + 2\mu\,\overset{\leftrightarrow}{d}, \tag{12}$$

or introducing tensor $stackrel{\leftrightarrow}p = -\ \overset{\leftrightarrow}{t}$, following Stokes [Stokes (1845)]:

$$\overset{\leftrightarrow}{p} = p\,\overset{\leftrightarrow}{I} - 2\mu\,\overset{\leftrightarrow}{d} + \left(\frac{2}{3}\mu - \kappa\right) I_d\,\overset{\leftrightarrow}{I}, \tag{13}$$

further generalization of the wall stress definition is achieved.

2.3 Transpiration effects

In 1846 and 1849 Graham [Graham (1846,1849)], and later in 1879 Reynolds [Reynolds (1879)], observed phenomena, today commonly known after Reynolds the transpiration effects. Transpiration effect manifests itself as a countercurrent at the wall to the bulk flow. That is, while the gradient between the inlet and the outlet of a microtube generates the flow in the opposite to the gradient direction, the transpiration occurs as the counter flow at the fluid-solid interface. When spoken of Graham observed transpiration, we speak of concentration transpiration. The "wall flow" occurs from the region of a lower concentration to the region of a higher concentration of a given constituent. When spoken of Reynolds observed transpiration, we speak of thermal transpiration, i.e. the flow from region of a lower temperature to the region of a higher temperature, also at the fluid-solid interface. Taking into account the transpiration effects, an also accounting for the pressure transpiration, we achieve a more general form of the friction force definition in a form:

$$\vec{f} = \nu(\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}) - (c_{s,\varpi}\ \mathrm{grad}_s\varpi + c_{s,\theta}\ \mathrm{grad}_s\theta + c_{s,c}\ \mathrm{grad}_s c), \tag{14}$$

where $c_{s,\varpi}$ and $c_{s,c}$ are the pressure and concentration transpiration coefficients, respectively, and $c_{s,\theta}$ is the Reynolds thermal transpiration coefficient.

2.4 Generalised boundary force condition

Given the, already defined in the previous subsection, contributions to the boundary friction force, the FFMI PASci team proposes the following constitutive equations of a generalized boundary force as a sum of friction force and the mobility force

[Badur, Karcz, and Lemanski (2011)]. Friction forces account for the medium interactions with the solid wall material. The division to mobility and friction terms allows the description of the generalized boundary force in a form:

$$\vec{f} = \vec{f}_f + \vec{f}_m, \tag{15}$$

where $_f$ index corresponds to the friction forces, and $_m$ index - to mobility forces. Both forces may be defined as follows:

$$\vec{f}_f = f_{static}N\frac{\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}}{|\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}|} + \nu(\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}) + f_k(\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall})^2\frac{\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}}{|\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}|}, \tag{16}$$

for the friction force, and:

$$\vec{f}_m = -(c_{s,\varpi}\ \mathrm{grad}_s\varpi + c_{s,\theta}\ \mathrm{grad}_s\theta + c_{s,c}\ \mathrm{grad}_s c + c_{s,\phi}\ \mathrm{grad}_s\phi + c_{s,x}\ \mathrm{grad}_s x), \tag{17}$$

for the mobility force. In the last equation for the mobility forces, there exist five gradients. Those are: concentration gradient for c symbol, electric potential gradient for ϕ symbol, pressure gradient for ϖ symbol, thermal gradient for θ symbol, phase transition progress gradient for x symbol. The given definition of the boundary force treats the subject in the most general form, that in some special cases may be simplified.

As a test of the model applicability, a comparison with experimental results, acquired by [Pitakarnnop, Varoutis, Valougeorgis, Geoffroy, Baldas, and Colin (2010)], was made. Since the experimental setup provides isothermal conditions for laminar monoatomic gas flow (helium and argon), the model could be simplified to only account for the velocity slip. In this case, the model would be of a form:

$$f_{static}N\frac{\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}}{|\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}|} + \nu(\vec{\mathrm{v}} - \vec{\mathrm{v}}_{wall}) = \mu\frac{\partial\vec{\mathrm{v}}}{\partial n}. \tag{18}$$

Since the $f_{static}N$ parametre is of unknown form or value, we decided to omit its discussion for the time being. Hence we achieved a striking resemblence to the standard Maxwell model. Thus the comparison with the results for Maxwell model was also performed:

$$\vec{\mathrm{v}} = \frac{\mu}{\nu}\frac{\partial\vec{\mathrm{v}}}{\partial n} = l_s\frac{\partial\vec{\mathrm{v}}}{\partial n}. \tag{19}$$

The numerical results are presented in Fig. 1. It is readily seen that both models give approximately similar results, although the FFMI PASci model seems to be more consistent, independently on the flowing medium. As can be seen for helium, the Maxwell model is less reliable than for argon. FFMI PASci doesn't suffer from such a drawback, and gives similar agreement regardless the gas.

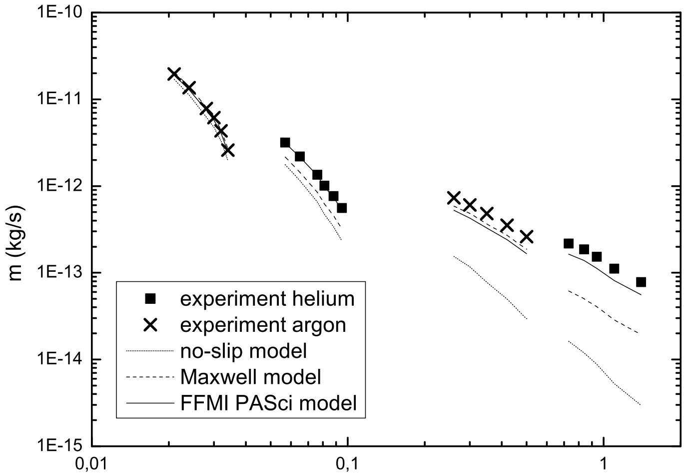

Figure 1: The mass flow rate [kg/s] versus Knudsen number for numerical simulation compared with experimental data provided in [Pitakarnnop, Varoutis, Valougeorgis, Geoffroy, Baldas, and Colin (2010)]

3 Temperature and concentration jump

Aside from the transport enhancement, due to wall effects manifesting themselves strongly particularily in the wall dominated flows, i.e. where characteristic length scale of the channel (hydraulic diametre) is of a comparable order of magnitude as the mean free path of a fluid molecules, there are also inequalities in thermal and concentration fields in the direction normal to the boundary. Those inequalities commonly referred to as jumps, were investigated in literature [Lewandowski, Ochrymiuk, and Czerwinska (2011); Jebauer and Czerwinska (2007); Xu and Ju (2005)].

3.1 Temperature jump model

It is very important to note at the very beginning, that the temperature jump should not be mistaken with the thermal transpiration. Since the latter influences flow enhancement, the former is connected with the normal to the wall inequality (which obviously to some extent may also have an effect on the flow field - but not as a prime cause), or interpreted as inequality of solid wall and fluid temperature. Proposed in 1896 by von Smoluchowski [von Smoluchowski (1910)] model introduces a characteristic length scale l_θ defined as the jump length, which is connected with the Stokes heat flux model [Stokes (1851)] as follows:

$$h(\theta - \theta_{wall}) + \vec{q}\cdot\vec{n} = 0, \tag{20}$$

where heat flux is defined by Fourier law [Fourier (1878)]:

$$\vec{q} = \lambda \ \mathrm{grad}\theta. \tag{21}$$

The temperature jump length was defined by Smoluchowski to be:

$$l_\theta = \frac{\lambda}{h}. \tag{22}$$

Generalized form of the boundary condition given by FFMI PASci has then a form:

$$\begin{aligned}\partial_t(c_{p,s}\theta_s) + \mathrm{div}_s(c_{p,s}\theta_s\vec{\mathrm{v}}_{s||}) - \theta_s I_b \vec{\mathrm{v}}_s\cdot\vec{n} + \mathrm{div}_s(\lambda_s \mathrm{grad}_s\theta_s) +\\ + h(\theta - \theta_{wall}) + \vec{q}\cdot\vec{n} = 0.\end{aligned} \tag{23}$$

3.2 Concentration jump model

In case of the flow of a fluid mixture an effect of concentration jump many occur, particularily when the reacting mixture is considered, and channel walls have catalytic properties. Thus the discontinuity of concentration may take place in the direction normal to the boundary. The model for the concentration boundary condition proposed by Lewis in 1924 was [Lewis and Whitman (1924)]:

$$\alpha(c - c_{wall}) + \vec{j}\cdot\vec{n} = 0, \tag{24}$$

where constituent flux is defined according to Fick's diffusion law [Fick (1855)]:

$$\vec{j} = D \ \mathrm{grad}c. \tag{25}$$

The closure for a corresponding concentration jump was propodsed in literature to be defined as:

$$l_c = \frac{D}{\alpha}. \tag{26}$$

Then the generalized form of the boundary condition of FFMI PASci is:

$$\begin{aligned}\partial_t(\rho_s c_s) + \mathrm{div}_s(\rho_s c_s\vec{\mathrm{v}}_{s||}) - c_s I_s \vec{\mathrm{v}}_s\cdot\vec{n} + \mathrm{div}_s(D_s \mathrm{grad}_s c_s) +\\ + \alpha(c - c_{wall}) + \vec{j}\cdot\vec{n} = 0,\end{aligned} \tag{27}$$

which is analogous to the definition for the temperature jump.

4 Summary

In the paper the form of the boundary condition model derived in FFMI PASci has been described. It was shown, that more than velocity slip may account for the flow enhancement phenomenon, i.e. the concentration, thermal, pressure, electric charge or phase progress gradients may have considerable impact on the flow behaviour. Aside from the cocurrent and countercurrent influences observed in the micro- and nanoflows, there exists a class of phenomenae enacting on the temperature and concentration fields manifesting themselves as temperature and concentration jumps, respectively, in the direction normal to the solid-fluid interface (or any two-phase interface). These discontinuities are non-negligible due to strong wall domination in the micro- and nanoflows. Further experimental and theoretical investigation in this field is also required to establish the form and value of the model's parametres. Along with the mentioned merits, the model provides a good physical interpretation of all the terms, however experimental research is required for confirmation of the modelling assumptions.

The model has proven to be better suited in computing microflows compared with the standard Maxwell model. The model's consistency is confirmed in a wide range of Knudsen numbers.

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