

The Model of Mass Transfer Intensification in Channels Using Nanowires inside and Nanostructures on the Wall

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Abstract. The gas and liquid mass transfer intensification is studied using nanowires placed in the flow as well as nanostructures organized on the channel wall. The results of the study can be applied to a drag reduction of the gas and liquid transport in channels. The model of drag reduction is developed using the set of submicronwires placed into the flow. On the wires surface the gas slippage in Knudsen layer is observed. The slippage results in a mass transfer intensification. The sets of wires placed near the channel axis of symmetry as well as placed close to the channel wall are analyzed for both types of channel surface that are smooth or have the submicron roughness. The slip boundary condition on the surface of a submicron wire and the subsequent averaging procedure over the set of wires are applied to find the intensity of gas slippage as a function of number density of wires distribution as well as of wires shape. The results of numerical simulation of gas transport under a given pressure drop in channels demonstrate the drag reduction up to 300 percent.

1. Introduction

The experimental study of convective and diffusive mass transfer in nanotubes [1, 2] demonstrated the intensification compared to tubes of micron diameter. The numerous application of nanowires are found in [3, 4]. The recent technology allow to obtain the sets of nanowires which diameter is one meter and the length is up to 10m. Let us note that the free pass length of gas molecules in the Knudsen layer close the wire surface can lie in the interval of 10 to 70 that causes the significance of the slippage effect. The problem of drag reduction for liquid transport was studied in [5–7] where numerous references can be found, however, a gas transport was not considered. Reducing the drag of marine vehicles via gas lubrication has long been practiced by injecting gas bubbles or creating a cavitation gas pocket [8] and reached a significant drag reduction (~ 95%) at high Reynolds number flow [9,10]. Since the gas film (or bubbles) does not stay on the solid surface by nature, however, these methods should continue supplying the gas with additional energy, overshadowing the benefit of drag reduction and limiting applications. The prospect of retaining the gas without energy input has been driving the recent explosive interest in superhydrophobic (SHPO) surfaces – a rough surface of a hydrophobic material. Surface roughness generally increases the skin-friction drag in turbulent boundary layer (TBL) flows [11] except for very few specific conditions [12]. However, if the hydrophobic roughness of the SHPO surface retains microscale air pockets and thus maintains a plastron, the resulting slip flow may bring an appreciable drag reduction. Recent establishment in the slips and drag reductions obtained on engineered SHPO surfaces in laminar flows [13–15] have heightened the anticipation that someday an appreciable reduction can be reliably obtained in TBL



flows as well [16,17]. Experimental data [10] demonstrates the bigger skin drag reduction for the smaller size of pitch on ultrahydrophobic surface. This result motivated us to consider submicron structure at channel surface filled with a gas. In the present paper the model for gas transport intensification using sets of nanowires is suggested. Close to the wire surface the Knudsen layer causes the gas slippage that intensifies the mass transfer. The numerical simulation of unsteady axially-symmetric flow in a tube for various sets of wires placed in the center of the flow as well as close to the wall surface are analyzed. The slip boundary conditions [18] were applied. The models of gas slippage in Knudsen layers [19, 20] appears to be in good agreement with experimental data. The results of drag reduction using the nanowire sets were reported in [21]. The application of submicron cavities on the channel surface are discussed in [22].

2. The gas flow with outer velocity $U = U_{ex}$ in microchannel over a nanowire

We consider firstly the analytical solution for outer flow problem over a nanowire in the microchannel as follows

$$\frac{1}{R} \frac{\partial}{\partial R} \left(\mu_g R \frac{\partial U}{\partial R} \right) = P_x, \quad R_0 < R < R_1.$$

$$-\mu_g U'(R_0) = B_u U(R_0) \text{ and } U(R_1) = U_{ex}.$$

Where the dimensional variables are used. We rewrite the microscale problem for dimensionless variables as follows

$$r = R / R_1, \quad u = U / U_{ex}, \text{ and } \text{Re}_{loc} = \frac{U_{ex} R_1 \rho_g}{\mu_g}$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{1}{\text{Re}_{loc}} r \frac{\partial u}{\partial r} \right) = p_x, \quad r_0 < r < 1, \quad \frac{-1}{\text{Re}_{loc}} u'(r_0) = b_u u(r_0), \text{ and } u(1) = 1.$$

Let u_{\max} be the maximal gas velocity. Our numerical computation of unsteady Quette flow shows that maximal velocity for steady state takes place on the wire surface. Denoting

$$k = \frac{1}{2} \left(1 + \frac{1}{u_{\max}} \right) \text{ and } u(r_*) = \frac{1}{2} (1 + u_{\max}).$$

We arrive at $p_x = -\frac{4}{\text{Re}_{loc}} u_{\max} \psi$, where $\psi = (1 - k) / r_*^2$.

3. Gas flow in macrochannel with a set of nanowires

Consider now the gas flow in a macro channel with placed inside of it a set of submicronwires. Let V_{meso} be the mesovolume whose diameter is much less than the diameter of macrochannel, however, the diameter is much more as compared to diameter of the wire. In subsequent computation the mesovolume is chosen as computational grid finitevolume as usual. Using the average of micro pressure gradient over the mesovolume, we arrive at

$$-J_{slip}^{macro} = \frac{1}{V_{meso}} \int_S p_x dS = \frac{1}{V_{meso}} \sum_j \int_{S_j} p_x dS = \frac{1}{V_{meso}} \sum_j S_j \hat{p}_{jx},$$

where summation over all wire surfaces is assumed. Denoting by n the number density of the wire set, we obtain the macroslippage intensity as follows

$$A_u = \frac{4nS^{mic}}{V_{meso} Re_{loc}} \text{ and } S^{mic} = 2\pi r^{mic} L^{mic}; \text{ where } r^{mic} \text{ and } L^{mic} \text{ are wire radius and length respectively.}$$

In common case of 3-d gas flow the slippage vector is $\vec{J}_{slip}^{macro} = A_u \mathbf{u}$. The momentum conservation equation reads

$$\frac{\partial \chi \rho \mathbf{u}}{\partial t} + \nabla \cdot (\chi \rho \mathbf{u} \mathbf{u}) + Ma^{-2} \nabla p = Re^{-1} \nabla \cdot \boldsymbol{\tau} + \vec{J}_{slip}^{macro}$$

$$\boldsymbol{\tau} = \mu \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right]$$

4. Gasflow in a channel which surface retains microscale air pockets

We consider a gas flow in a channel with submicron pockets filled with gas. The averaging procedure over the mesovolume that is similar to the written above, allows us to represent the boundary slip condition in the form

$$\mu_g \frac{\partial \hat{U}}{\partial R} = \hat{B}_u \hat{U}, \text{ where } \hat{B}_u = \frac{S_b n}{S \cdot R_b}, \text{ or } \hat{B}_u = \frac{n}{r_w}, S_b = 2\pi R_b L, S = 2\pi r_w L.$$

The values R_b, L_b denote radius and length of air pocket respectively and \hat{U} is the mean flow velocity in the mesovolume.

5. The results of masstransfer simulation in the channel with a nanowire ensemble inside

We consider the nanowire set of radius r_c and length l_s placed on the channel axis at $x = x_s$. The slippage intensity is defined using the functions

$$f_x(x) = \begin{cases} 1, & x_s < x < l_s \\ 0, & l_s \leq x \leq L \end{cases} \text{ and } f_{r0}(r) = \begin{cases} 1, & 0 < r < r_c \\ 0, & r_c \leq r \leq 1 \end{cases}, \quad (1)$$

$$\vec{J}_{slip}^{macro} = A_u f_{r0}(r) f_x(x) \mathbf{u} \sqrt{p\rho}$$

Along with we consider two nanowire sets of radius r_c and length l_s placed on the channel axis at $x = x_s$ and $x = x_s + 2l_s$. The slippage intensity is defined using the functions

$$f_{1x}(x) = \begin{cases} 1, & x_s < x < l_s \\ 0, & (l_s \leq x \leq L) \cap (0 \leq x \leq l_s) \end{cases} \text{ and } f_{2x}(x) = \begin{cases} 1, & x_s + 2l_s < x < 3l_s \\ 0, & (3l_s \leq x \leq L) \cap (0 \leq x \leq x_s + 2l_s) \end{cases} \quad (2)$$

$$\vec{J}_{slip}^{macro} = A_u f_{1x}(x) f_{2x}(x) \mathbf{u} \sqrt{p\rho}$$

The results of simulation refer to $x_s = 0.05, l_s = 0.5, L = 3$.

We obtained the more intensive masstransfer for one nanowire ensemble model (1) compared to two nanowire ensembles model (2). The reason is the gap between nanowires sets (2).

Our computation shows that the bigger value of the Reynolds number the bigger maximal value of the massflow for the same instant of time and more intensive masstransfer.

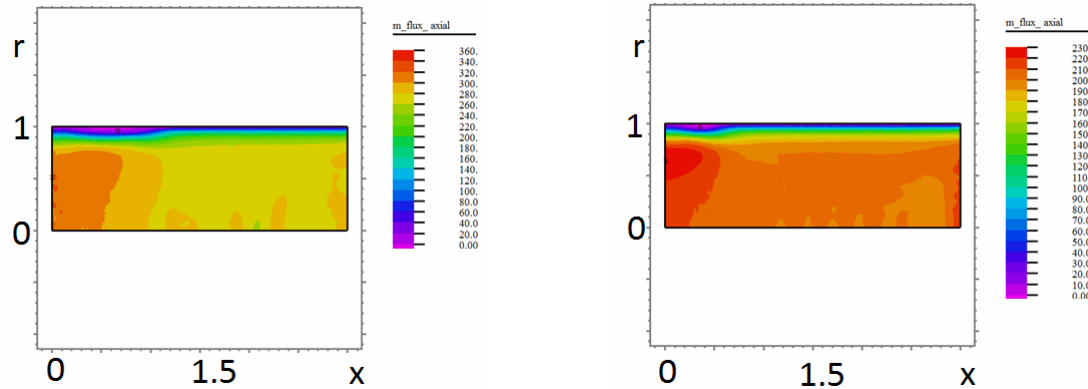


Figure 1. Comparison one nanowire ensemble $L_s=1$ and two ones of $L_s=0.5$ each. Mass flow in the channel with a set of two nanowire ensembles of radius $r_c = 0.1$ placed in the tube centre is presented. The massflow distribution is shown at time instant $t = 0.166$ and $Re = 1$ for one shim of length $l_s = 1$ at $x_s = 0.05$ sec (1) (left) and two shims of length $l_s = 0.5$ at $x_s = 0.05$, $x_s = 1.05$ sec (2) (right).

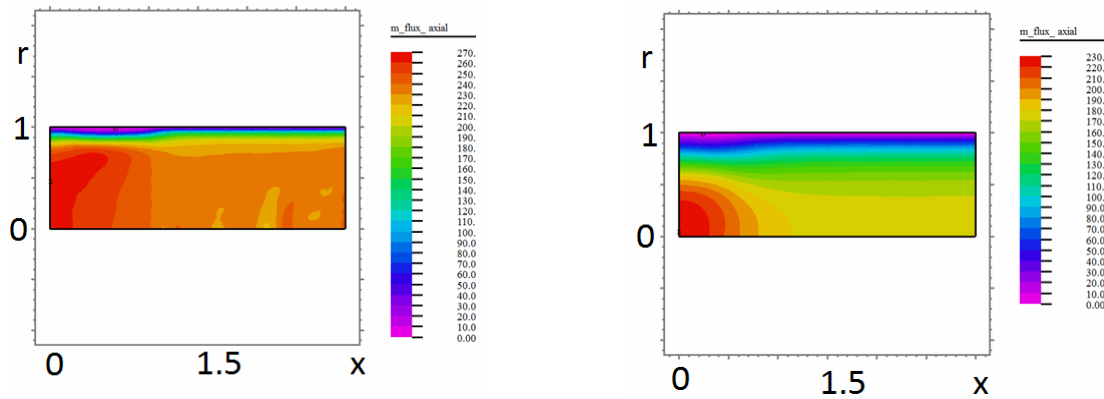


Figure 2. Massflow in the channel with two sets of nanowires of radius $r_c = 0.1$ placed in the tube centre is presented. The massflow distribution is shown at time instant $t = 0.15$ for $Re = 1$ (left) and $Re = 0.1$ (right).

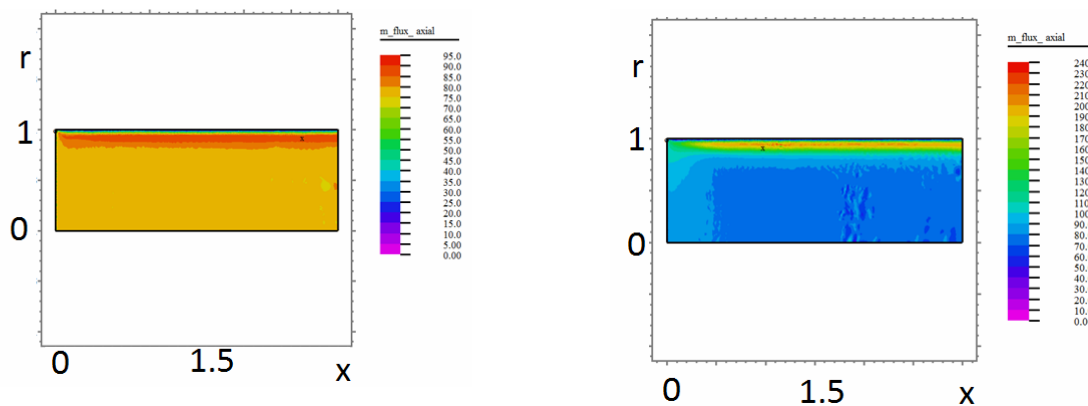


Figure 3. Massflow of gas in the channel with a set of nanowires of radius $r_c = 0.1$ attached to the wall is presented. The massflow distribution is shown at time instant $t = 0.086$ for $Re = 10$ and $A_u = 150$ (left) and $A_u = 750$ (right).

The transfer intensification coefficient is defined as $K = Q / Q_0$, $Q = 2\pi \int_0^1 u(t, x, r) \rho r dr$. The results of numerical simulation using the sets of nanowires of radius r_c as well as using gasslippage on the channel surface due to organized submicron air pockets on the channel wall are as follows. The value Q_0 refers to the integral mass flow when no slippage occurs. In the columns, 1, 2 the results of $Q(L, t)$ computation refer to the flow with a set of wires attached to the channel wall.

$$A_u = 0.001, B_u = 1, r_c = 0.1, K = 2.93$$

$$A_u = 750, B_u = 1, r_c = 0.1, K = 3.95$$

6. Conclusion

Microanalysis of flow near nanowire and subsequent averaging mass transfer over the set of nanowires placed in the flow, enables to obtain the value of slippage intensity, which depends on number density of wires as well as on the wires shape and size. The numerical simulation of the unsteady gas mass transfer in the channel flow with axial symmetry has been carried out in a wide range of similarity parameters. The results show significant mass transfer intensification (up to 300 percent) due to the set of nanowires placed in the center of channel as well as for wires attached to the channel surface. The organized surface structures on the channel wall provide the gasslippage in the Knudsen layer near the wall. The remarkable mass transfer intensification has been found using the submicron pockets filled with gas on the channel wall.

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References

- [1] Karnidakis G A and Aluru N 2005 Microflows and nanoflows. Fundamentals and Simulation (Foreword by Chih-Ming Ho) *Interdisciplinary Applied Math.* 29. Springer Science+Business Media, Inc., p 817
- [2] Holt J K, Park H G, Wang Y S M, Artyukhin A B, Grigoropoulos C P, Noy A and Bakajin O 2006 Fast mass transport through sub-2-nanometer carbon nanotubes *Science* **312** pp 1034–1037
- [3] Aktas E O, Ozgur H D, Enes K and Mehmet 2011 *Nature Materials*. **10** pp 494–501
- [4] Filippov G A, Saltanov G A and Kukushkin A N. Hydrodynamics and heat mass transfer in the presence of polymer molecular wires 1981 (in Russian) *Moscow Energoatomizdat* p 184
- [5] Ceccio S L 2010 Friction drag reduction of external flows with bubble and gas injection *Annu. Rev. Fluid Mech.* **42** pp 183–203
- [6] Lay K A, Ryo Y, Simo M, Perlin M and Ceccio S L 2010 Partial cavity drag reduction at high Reynolds numbers *J. Ship Res.* **54** pp 109–119
- [7] Hyungmin P, Guangyi S and Chang-Jin K. 2014 Superhydrophobic turbulent drag reduction as a function of surface grating parameters *Journal of Fluid Mechanics* Vol. 747, May 2014, pp 722–734
- [8] Walsh M J 1982 Turbulent boundary layer drag reduction using griblets *AIAA Paper* 0169
- [9] Jimenez J 2004 Turbulent flows over rough walls *Annu. Rev. Fluid Mech.* **36** pp 173–196
- [10] Jung Y C and Bhushan B 2010 Biomimetic structures for fluid drag reduction in laminar and turbulent flows *J. Phys: Condens. Matter* **22** 035104
- [11] Ou J, Perot B and Rothstein J P 2004 Laminar drag reduction in microchannels using ultrahydrophobic surfaces *Phys. Fluids* **16** pp 4635–4643
- [12] Choi C H and Kim, C J 2006 Large slip of aqueous liquid flow over a nanoengineered superhydrophobic surface *Phys. Rev. Lett.* **96** 066001
- [13] Rothstein J P 2010 Slip on superhydrophobic surfaces *Annu. Rev. Fluid Mech.* **42** pp 89–109
- [14] Samaha M A, Tafreshi H V and Gad-el-Hak M 2012 b Superhydrophobic surfaces: from the

- lotus leaf to the submarine *C.R. Mec.* **340** pp 18–34
- [15] Bocquet L and Lauga E 2011 A smooth future? *Nature Mater.* **10** p 334
- [16] Lee C, Choi C H, and Kim C J 2008 Structured surfaces for a giant liquid slip *Phys. Rev. Lett.* **101**, 064501
- [17] Lee C, Choi C H and C-J Kim 2008 *Phys. Rev. Lett.* **101**, 064501
- [18] Lee A and Kim H Y 2014 Does liquid slippage within a rough channel always increase the flow rate? *Phys. Fluids*, **26**, 072002
- [19] Markov A A 2014 Jump-Slip simulation technique for combustion in submicron tubes and sub-micron pores *Computers and Fluids* **99 C**, pp. 83-92
- [20] Markov A A, Hobosyan M A and K S Martirosyan K S 2015 Ferrite Synthesis Simulation via Carbon Combustion using Slip, Temperature, and Concentration Gas Species Jump at Pore Surface *Physical-Chemical Kinetics in Gas Dynamics* **16** (1)
<http://chemphys.edu.ru/issues/2015-16-1/articles/506/>
- [21] Markov A A, Hobosyan M A and Martirosyan K S 2015 Simulation of heat and masstransfer in pores as applied to synthesis of magnesium–zinc and nickel–zinc ferrite nanoparticles, *Nanomechanics Science and Technology: An International Journal* **6**(3), pp. 1–14
- [22] Markov A A 2016 On heat- and masstransfer in channels with setof nanowires. *Proc. XIIInternConf. NPNJ* pp. 95-97. ISBN 978-5-4316-0300-6
- [23] Aleksin V A and Markov A A 2015 Intensification of mass transfer in laminar and turbulent channelflows by applying submicron cavities on the channel wall surface *Nanomechanics Science and Technology: An International Journal* **6**(4), pp. 319-334