EVALUATION OF ELECTRO-OSMOTIC FLOW IN A NANOCHANNEL VIA SEMI-ANALYTICAL METHOD

by

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In this paper, equations due to anion and cation distributions, electrical potential and shear stress profiles in a nanochannel are formed for 1-D electro-osmotic flow, and solved by homotopy perturbation method. Results are compared with numerical solutions.

Key words: *nanochannel, electro-osmotic flow, electrical double layer, homotopy perturbation method; numerical solution*

Introduction

In recent decades, after introducing micro- and nanofabrication technologies, several possibilities in the case of micro- and nanofluidic devices have been invented. This idea has been followed by some modern technologies such as Lab-on-a-Chip.

One of the most important subsystems of the micro- and nanofluidic devices is their passage or "Micro- and Nanochannel". Nanochannel term is referred to channels with hydraulic diameter less than 100 nanometers [1]. By decrease in size and hydraulic diameter some of the physical parameters such as surface tension will be more significant while they are negligible in normal sizes.

Concentrating surface loads in liquid – solid interface makes the electrical double layer (EDL) to be existed. If the loads are concentrated in the end of nanochannels, a potential difference will be generated that forces the ions in the nanochannel. However, induced electric field is discharged by electric conduction of the electrolyte.

The first significant work that was done in the literature belongs to 1870 that Helmholtz introduced the EDL. According to this finding, flow and electricity parameters for electro-osmotic transport were detected. Electroosmotic processes have been utilized since 1930s. Modern theoretical progresses in the case of electro-osmotic flow can be found in [2-6]. Burgreen and Nakache [2] and Oshima and Kondo [3] studied the flow between two parallel

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plates. Also, Rice and Whitehead [4], Lu and Chan [5] and Ke and Liu [6] studied the flow in capillary tube. Recently these kinds of problems have been analyzed by some researchers using analytical methods [7-9]. By the way, some papers consider curvilinear co-ordinates in this case [10, 11]. Also, all of them studied the problem with existence of the pressure gradient while in the modern applications, the pressure gradient can be eliminated and consequently, solving the problem considering this fact is necessary. In this paper, it will be studied in a nano-channel by homotopy perturbation method (HPM) and next, results will be compared by numerical one.

Mathematical modeling

For a long and wide channel as shown in fig. 1, in [12], equations governing the electro-osmotic phenomena for rectilinear co-ordinates system have been investigated.

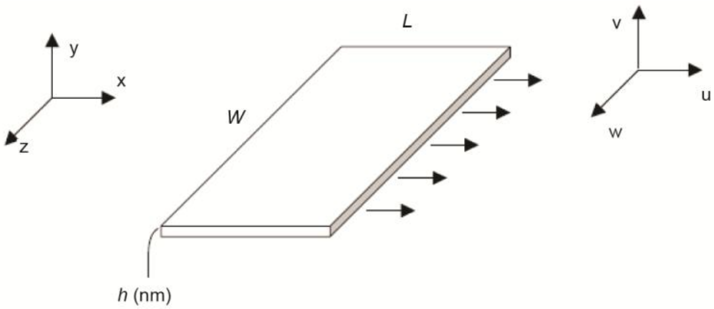

Figure 1. Geometry of 1-D channel *W* □ *h*, *L* □ *h*

$$\varepsilon^2 \frac{\mathrm{d}^2\varphi}{\mathrm{d}y^2} = -\beta(x_+ - x_-) \tag{1}$$

$$\varepsilon^2 \frac{\mathrm{d}^2 u}{\mathrm{d}y^2} = -\beta(x_+ - x_-), \quad \tau = \frac{\partial u}{\partial y} \tag{2}$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{\mathrm{d}x_+}{\mathrm{d}y} + x_+ \frac{\mathrm{d}\varphi}{\mathrm{d}y}\right) = 0 \tag{3}$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{\mathrm{d}x_-}{\mathrm{d}y} - x_- \frac{\mathrm{d}\varphi}{\mathrm{d}y}\right) = 0 \tag{4}$$

These equations represent Poisson-Boltzmann, Navier-Stokes, and conservation of species equations, respectively, x_+ is the mole fraction of cation, x_- – the mole fraction of anion, u – the dimensionless velocity, β – the ionic strength, ε – the Debye-Huckel length, τ – the shear stress and φ – the dimensionless potential. The boundary conditions are:

$$\varphi = 0 \quad y = 0 \quad \text{and} \quad y = 1 \tag{5}$$

$$u = 0 \quad y = 0 \quad \text{and} \quad y = 1 \tag{6}$$

$$x_+ = x_+^0 \quad y=0 \quad \text{and} \quad y=1 \tag{7}$$

$$x_- = x_-^0 \quad y=0 \quad \text{and} \quad y=1 \tag{8}$$

With discrete modeling and simplification of eq. (4):

$$X_- \frac{d^2 X_-}{dy^2} - \left(\frac{dx_-}{dy}\right)^2 + \frac{X_+^0 \cdot X_-^0 \cdot \beta}{\varepsilon^2} X_- - \frac{\beta}{\varepsilon^2} X_-^{\;3} = 0 \tag{9}$$

where x_+ and x_- are the mole fraction of cation and anion at the channel wall, respectively.

Homotopy perturbation method

To illustrate the basic ideas of this method [13], we consider the following equation:

$$A(u) - f(r) = 0, \qquad r \in \Omega \tag{10}$$

With the boundary condition:

$$B\left(u, \frac{\partial u}{\partial n}\right) = 0, \qquad r \in \Gamma \tag{11}$$

where A is a general differential operator, B – a boundary operator, $f(r)$ – a known analytical function, and Γ is the boundary of the domain Ω. A can be divided into two parts which are L and N, where L is linear and N is non-linear. Equation (10) can therefore be rewritten as:

$$L(u) + N(u) - f(r) = 0, \quad r \in \Omega \tag{12}$$

Homotopy perturbation structure is shown as follows:

$$H(v,p) = (1-p)\ \ L(v) - L(u_0)\ \ + p\ \ A(v) - f(r)\ \ = 0 \tag{13}$$

where
$$v(r,p):\ \Omega \times\ 0,1\ \to R \tag{14}$$

In (10), $p \in [0, 1]$ is an embedding parameter and u_0 is the first approximation that satisfies the boundary condition. We can assume that the solution of (10) can be written as a power series in p, as following:

$$v = v_0 + pv_1 + p^2 v_2 + \ldots \tag{15}$$

And the best approximation for solution is:

$$u = \lim_{p\to 1} v = v_0 + v_1 + v_2 + \ldots \tag{16}$$

Solving problem by homotopy perturbation method

By assuming the convenient first guess, the following solution will be achieved:

$$X_-(y) = -1.026419033 \cdot 10^{-17} e^{29.976386633y} - \\ - 0.0001071282146 e^{-29.97639633y} + 0.002647128214 \tag{17}$$

$$X_{+}(y)= \\ =\frac{7.01\cdot 10^{-6}}{-1.026419033\cdot 10^{-17}\mathrm{e}^{29.97638633y}-0.0001071282146\mathrm{e}^{-29.97638633y}+0.002647128214} \tag{18}$$

$$\varphi(y)=u(y)= \\ =\ln\frac{-1.026419033\cdot 10^{-17}\mathrm{e}^{29.97638633y}-0.0001071282146\mathrm{e}^{-29.97638633y}+0.002647128214}{0.00254} \tag{19}$$

$$\tau(y)= \\ =\frac{-1.211351711\cdot 10^{-13}\mathrm{e}^{29.97638633y}+1.264297932\mathrm{e}^{-29.97638633y}}{-4.041019814\cdot 10^{-15}\mathrm{e}^{29.97638633y}-0.0421764244\mathrm{e}^{-29.97638633y}+1.042176462} \tag{20}$$

By comparing the results of numerical simulations and HPM solution, tabs. 1-2 can be developed.

Table 1. The results of HPM and NM methods for $X_{-}(y)$ and $X_{+}(y)$

	$X_{-}(y)$			$X_{+}(y)$		
y	HPM	NM	Error	HPM	NM	Error
0.00	0.0025400000	0.0025400000	0.0000000000	0.0027598425	0.0027598425	0.0000000000
0.05	0.0026164040	0.0026163936	0.0000000104	0.0026792605	0.0026792501	0.0000000104
0.10	0.0026394854	0.0026386954	0.0000007900	0.0026566158	0.0026558258	0.0000007900
0.15	0.0026462961	0.0026451261	0.0000011700	0.0026501572	0.0026489872	0.0000011700
0.20	0.0026485032	0.0026469732	0.0000015300	0.0026483079	0.0026467779	0.0000015300
0.25	0.0026492830	0.0026475030	0.0000017800	0.0026477779	0.0026459979	0.0000017800
0.30	0.0026497750	0.0026476550	0.0000021200	0.0026476259	0.0026455059	0.0000021200
0.35	0.0026496205	0.0026476985	0.0000019220	0.0026475824	0.0026456604	0.0000019220
0.40	0.0026496332	0.0026477110	0.0000019222	0.0026475699	0.0026456477	0.0000019222
0.45	0.0026497565	0.0026477145	0.0000020420	0.0026475664	0.0026455244	0.0000020420
0.50	0.0026497074	0.0026477152	0.0000019922	0.0026475657	0.0026455735	0.0000019922
0.55	0.0026497323	0.0026477145	0.0000020178	0.0026475664	0.0026455486	0.0000020178
0.60	0.0026496102	0.0026477110	0.0000018992	0.0026475699	0.0026456707	0.0000018992
0.65	0.0026497988	0.0026476985	0.0000021002	0.0026475824	0.0026454822	0.0000021002
0.70	0.0026498402	0.0026476550	0.0000021852	0.0026476259	0.0026454407	0.0000021852
0.75	0.0026494902	0.0026475030	0.0000019872	0.0026477779	0.0026457907	0.0000019872
0.80	0.0026489900	0.0026469732	0.0000020168	0.0026483079	0.0026462911	0.0000020168
0.85	0.0026471136	0.0026451261	0.0000019876	0.0026501572	0.0026481696	0.0000019876
0.90	0.0026405723	0.0026386954	0.0000018769	0.0026566158	0.0026547389	0.0000018769
0.95	0.0026186136	0.0026163936	0.0000022200	0.0026792605	0.0026770405	0.0000022200
1.00	0.0025400000	0.0025400000	0.0000000000	0.0027598425	0.0027598425	0.0000000000

Conclusions

In this work, our main concern has been to study applicability of HPM in solving a non-linear singular differential equation. The example presented here is equations governing electro-osmotic flow inside a nano-channel. An approximation to the analytic solution was obtained by applying the HPM [14-23].

Table 2. The results of HPM and NM methods for φ (*y*) and τ (*y*)

	φ (*y*)			τ (*y*)		
y	HPM	NM	Error	HPM	NM	Error
0.00	0.0000000000	0.0000000000	0.0000000000	1.0379513814	1.0379513814	0.0000000000
0.05	0.0296328104	0.0296328000	0.0000000104	0.2973854548	0.2973854444	0.0000000104
0.10	0.0381213373	0.0381205473	0.0000007900	0.0852829529	0.0852821629	0.0000007900
0.15	0.0405558280	0.0405546580	0.0000011700	0.0244566839	0.0244555139	0.0000011700
0.20	0.0412542475	0.0412527175	0.0000015300	0.0070126127	0.0070110827	0.0000015300
0.25	0.0414546306	0.0414528506	0.0000017800	0.0020122653	0.0020104853	0.0000017800
0.30	0.0415123815	0.0415102615	0.0000021200	0.0005780234	0.0005759034	0.0000021200
0.35	0.0415286130	0.0415266910	0.0000019220	0.0001665761	0.0001646541	0.0000019220
0.40	0.0415333343	0.0415314121	0.0000019222	0.0000487264	0.0000468042	0.0000019222
0.45	0.0415347760	0.0415327340	0.0000020420	0.0000144287	0.0000123867	0.0000020420
0.50	0.0415349906	0.0415329984	0.0000019922	0.0000020058	0.0000000136	0.0000019922
0.55	0.0415347518	0.0415327340	0.0000020178	-0.0000103689	-0.0000123867	0.0000020178
0.60	0.0415333113	0.0415314121	0.0000018992	-0.0000449050	-0.0000468042	0.0000018992
0.65	0.0415287912	0.0415266910	0.0000021002	-0.0001625539	-0.0001646541	0.0000021002
0.70	0.0415124467	0.0415102615	0.0000021852	-0.0005737182	-0.0005759034	0.0000021852
0.75	0.0414548378	0.0414528506	0.0000019872	-0.0020084981	-0.0020104853	0.0000019872
0.80	0.0412547343	0.0412527175	0.0000020168	-0.0070090659	-0.0070110827	0.0000020168
0.85	0.0405566456	0.0405546580	0.0000019876	-0.0244535263	-0.0244555139	0.0000019876
0.90	0.0381224242	0.0381205473	0.0000018769	-0.0852802860	-0.0852821629	0.0000018769
0.95	0.0296350200	0.0296328000	0.0000022200	-0.2973832244	-0.2973854444	0.0000022200
1.00	0.0000000000	0.0000000000	0.0000000000	-1.0379513814	-1.0379513814	0.0000000000

A comparison of the results between numerical solution and HPM solution are given. It suggests that the HPM is accurate, reliable and easy to use. Furthermore, as it can be seen in tabs. 1 and 2, in some cases, the result that has been obtained from HPM has more consistency with numerical ones. The nearer to the nano-channel wall, as it can be easily seen, over 95% of the solution field, HPM results have consistency with numerical results. After all, we can accept HPM as well. HPM has its own weaknesses as well. The most important limitation in using HPM is finding first guess of a homotopic function v_0. Consequently, if first guess of the homotopic function is not approached correctly, solution will be kept on without any alarm. As a result, after simulation, validation with other methods is mandatory in order to avoid wrong approaches. As it has been mentioned, results in this paper are validated by numerical method.

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