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Assessment of the electroosmotic flow through a nano tube

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Abstract : Electroosmotic flow through a nano tube and nano channel has many applications in biomechanics and other sciences. Electroosmosis is the movement of solvent together with solute under an applied electric field. For solving of the Governing equations on Electroosmotic flow we can use some semi analytical methods such as Reconstruction of Variational Iteration Method (RVIM). Unlike perturbation method the RVIM is independent of small parameters. RVIM technique is a powerful and convenient algorithm in finding the approximate solutions for the linear and nonlinear equations. While RVIM is capable of reducing the size of calculation, it omits the difficulty arising in calculating nonlinear intricately terms. Also, it overcomes the difficulty of the Adomian polynomials by applying Laplace Transform and avoiding the use of Lagrange multiplier. In this paper, Poisson-Boltzmann equation has been investigated. This equation is employed in electrokinetic phenomena. Poisson-Boltzmann equation for a 30 nm diameter nano tube has been solved on the curvilinear coordinates. RVIM is applied and it is shown that accuracy and convergence of the results is good.

Keywords : Electroosmotic flow; Nano tube; Poisson-Boltzmann equation; Semi analytical solutions.

INTRODUCTION AND MATHEMATICAL MODELING

Recently, after introducing micro fabrication technologies, several possibilities in the case of micro fluidic devices have been invented. This idea has been expanded to nano fluidic devices and followed by some modern technologies such as Lab-on-a-Chip. One of the most important subsystems of the micro and nano fluidic devices is micro and nano Channel. Nano channel term is referred to channels with hydraulic diameter less than 100 nanometers[1]. Some of the physical parameters such as surface tension are negligible in normal sizes. By decreasing the size and hydraulic diameter, these physical parameters will be more significant. Concentrating surface loads in liquid – solid interface makes the EDL to be existed. If the loads are concentrated in the end of nano channels, 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. In 1870 according to the first significant work that was introducing the EDL by Helmholtz, flow and electricity parameters for electrokinetic transport were detected. Electroosomotic processes have been utilized since 1930s. Electroosmotic flow is commonly used in micro fluidic devices[2], soil analysis and processing[3].

Modern theoretical progresses in the case of electrokinetic flow can be found in[4-8]. Burgreen and Nakache[4] and Oshima and Kondo[5] studied the flow between two parallel plates. Also, Rice and Whitehead[6], Lu and Chan[7] and Ke and Liu[8] studied the flow in capillary tube. By the way, some papers consider curvilinear coordinates in this case[9,10]. 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, for small zeta potentials without pressure gradient will be studied based on the curvilinear coordinates in a nano tube by RVIM methods and next, results will be compared by analytical and numerical ones. Equations governing the electrokinetic phenomena for rectilinear coordinates system have been investigated[11,12]. Also these equations govern the nano tube electrokinetic phenomena in curvilinear coordinates system as follow, Figure 1[13]:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \varphi}{\partial r}\right)=\frac{-\beta}{\varepsilon^2}\left(X_p-X_m\right) \quad (1)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)=\frac{-\beta}{\varepsilon^2}\frac{\varepsilon_e E_0 R T}{F\mu U_0}\left(X_p-X_m\right) \quad (2)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\frac{\partial X_p}{\partial r}+\alpha X_p\frac{\partial \varphi}{\partial r}\right)\right]=0 \quad (3)$$

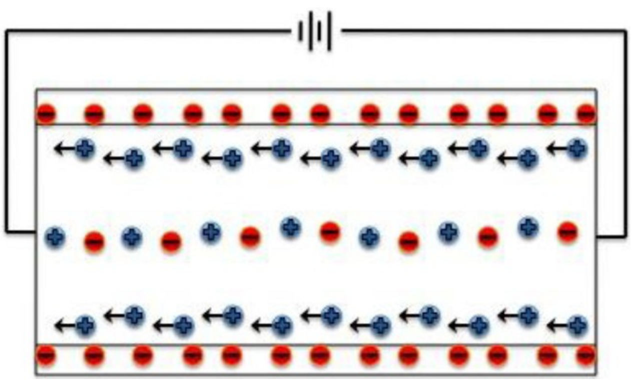

Figure 1 : Schematic of electroosmotic flow

$$\frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\frac{\partial X_m}{\partial r}-\alpha X_m\frac{\partial \varphi}{\partial r}\right)\right]=0 \quad (4)$$

Equations (1) to (4) represent the Poisson-Boltzmann, Navier-Stokes and conservation of species equations respectively. In these equations, r is dimensionless radius that is normalized by nano tube radius; u is dimensionless velocity that is normalized by free stream velocity U_0. β is ionic strength, q is the elementary charge and ε is Debye-Huckel parameter. ε_e is dielectric constant of water, ε_r is the relative permittivity of the solvent and ε_0 is the permittivity of free space. R is gas constant, T is temperature and F is Faraday constant. k_B is Boltzmann's constant, μ is dynamic viscosity and X is concentration ratio of cation (p subscript) and anion (n subscript). Also, φ is dimensionless potential that is normalized by zeta potential. And E_0 is the applied electric field. In this paper, it is assumed that, zeta potential is too small. Assuming

$\varepsilon=\sqrt{\dfrac{\varepsilon_r\varepsilon_0 k_B T}{\beta q}}$ and low concentrations, we have:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \phi}{\partial r}\right)=\frac{\phi}{\varepsilon^2},\ @\,r=0\Rightarrow\phi'=0 \text{ and } @\,r=1\Rightarrow\phi=1 \quad (5)$$

This is the simplified form of Poisson-Boltzmann Equation for diffuse layer in nano tube with small zeta potential and consequently, this paper main case study.

RVIM METHOD AND CONVOLUTION THEOREM

In this section, an alternative method for finding the optimal value of the Lagrange multiplier by the use of the Laplace transform will be investigated[14,15]. Suppose x is the independent variable; When the Laplace transform is applied to x as variable, definition of Laplace transform is

$$\mathrm{L}\ \{u(x,t);s\}=\int_0^\infty e^{-st}u(x,t)\,dt \quad (6)$$

$$\mathrm{L}\ \left\{\frac{\partial u}{\partial x},s\right\}=\int_0^\infty (e^{-sx}\frac{\partial u}{\partial x})\,dx=sU(s)-u(o) \quad (7)$$

$$\mathrm{L}\ \left\{\frac{\partial^2 u}{\partial x^2},s\right\}=s^2U(s)-su(o)-u_x(0) \quad (8)$$

$$U(s)=\mathrm{L}\ \{u(x);s\} \quad (9)$$

We often come across functions which are not the transform of known functions. But, by means of the convolution theorem, we can take the inverse laplace transform. The convolution of $u(x)$ and $v(x)$ is written as $u(x) \times v(x)$. It is defined as the integral of the functions after one is reversed and shifted.

If $U(s)$ and $V(s)$ are the Laplace transform of $u(x)$ and $v(x)$, respectively. Then $U(x) \times V(s)$ is the Laplace Transform of $\int_0^x u(x-\varepsilon)\cdot v(\varepsilon)d\varepsilon$ so we can take inverse Laplace Transform as below,

$$\mathrm{L}^{-1}\{U(s) * V(s)\} = \int_0^x u(x-\varepsilon)\cdot v(\varepsilon)d\varepsilon \quad \textbf{(10)}$$

To illustrate the concept of the RVIM, we consider the following general differential equation

$$L(u(x)) + N(u(x)) = f(x) \quad \textbf{(11)}$$

Where L and N are linear and nonlinear operators respectively. And $f(x)$ is the forcing term. To facilitate our discussion of RVIM, introducing the new function $h(u(x)) = f(x) - N(u(x))$ and considering the new equation, rewrite Eq. (11) as,

$$L(u(x)) = h(u,x) \quad \textbf{(12)}$$

Now, for implementation the RVIM technique based on new idea of Laplace transform, apply Laplace Transform on both sides of the Eq. (12). Now we introduce artificial initial conditions to zero for main problem, then left hand side of equation after transformation featured as

$$\mathrm{L}\{L(u(x))\} = U(s)P(s) \quad \textbf{(13)}$$

Where $P(s)$ is polynomial with the highest order derivative of the selected linear operator.

$$\mathrm{L}\{L(u(x))\} = U(s)P(s) = \mathrm{L}\{h(u,x)\} \quad \textbf{(14)}$$

$$U(s) = \frac{\mathrm{L}\{h(u,x)\}}{P(s)} \quad \textbf{(15)}$$

And suppose that $D(s) = \frac{1}{P(s)}$ and $\mathrm{L}\{h(u,x)\} = H(s)$. Using the convolution theorem we have

$$U(s) = D(s).H(s) = \mathrm{L}\{d(x) * h(u,x)\} \quad \textbf{(16)}$$

Taking the inverse Laplace transform on both sides of Eq. (16)

$$u(x) = \int_0^x d(x-\varepsilon)\cdot h(u,\varepsilon)d\varepsilon \quad \textbf{(17)}$$

Thus the following reconstructed method of variational iteration formula can be obtained

$$u_{n+1}(x) = u_0(x) + \int_0^x d(x-\varepsilon)\cdot h(u_n,\varepsilon)d\varepsilon \quad \textbf{(18)}$$

SOLVING PROBLEM BY RVIM METHOD

First, we consider Eq. (5), with the initial condition,

$$\varphi_0(r) = \varphi(0) = a \quad \textbf{(19)}$$

Considering Eq. (12) for this equation we have,

$$L(\varphi,r) = \frac{\partial\varphi}{\partial r} = \overbrace{\frac{\varphi}{\varepsilon^2} - \frac{\partial\varphi}{\partial r})}^{h(u,x)} \quad \textbf{(20)}$$

Applying Laplace Transform with respect to variable r to both sides of Eq. (20), one can get,

$$[s]\Phi(s) = \mathrm{L}\{h(\varphi(0),r)\} \quad \textbf{(21)}$$

$$\Phi(s) = \frac{\mathrm{L}\{h(\varphi,r)\}}{s} \quad \textbf{(22)}$$

Using the inverse Laplace Transform and convolution theorem, we have

$$\varphi(r) = \int_0^r h(\varphi,s)ds \quad \textbf{(23)}$$

So, in exchange with applying recursive algorithm, following relations are achieved

$$\varphi_{n+1}(r) = \varphi_0(r) - \int_0^r (\frac{\varphi_n(s)}{\varepsilon^2} - \frac{\partial\varphi_n(s)}{\partial s})ds \quad \textbf{(24)}$$

So we have,

$$\varphi_1(r) = a + 50\cdot a\cdot r^2 \quad \textbf{(25)}$$

$$\varphi_2(r) = a + 416.7\cdot a\cdot r^4 \quad \textbf{(26)}$$

$$\varphi_3(r) = a + 50\cdot a\cdot r^2 - 138.9\cdot a\cdot r^4 + 1388.9\cdot a\cdot r^6 \quad \textbf{(27)}$$

The above process is continuous.

To obtain the value of a, we substitute the boundary condition from Eq. (5) into $\varphi_i(r, a)$ at y=1. Solving $\varphi_i(a) = 1$, gives the value of a. This value is long that are not shown in this paper. By substituting obtained a, we can calculate the expressions of $\varphi_i(r)$. By comparing the results of this simulation TABLE 1 can be developed for 10th order RVIM[12].

Figures Plotted by RVIM are shown in Figure 2 to 5 in various coordinates. As shown in Figure 2, while we put the bigger amount of epsilon we have more potential. In increase of epsilon the angel of curve shown dimensionless potential increases. Figures 3 and 4 show the contours of these amounts in case of increase of epsilon as well. Also the spherical coordinate of potential plot is simulated in Figure 5. Meaningfully, the trends of increasing amount of the potential are obvious in Figures 3 to 5 same as Figure 3. Due to the definition of ε, Debye-Huckel parameter $\varepsilon = \sqrt{\frac{\varepsilon_r\varepsilon_0 k_B T}{\beta q}}$, we have a rise in the amount of the potential in increase of

TABLE 1 : Comparison of the results by the three different methods

r	RVIM Results	Numerical Results	HPM Results
0.0	0.00035	0.00000	0.00036
0.1	0.00037	0.00039	0.00046
0.2	0.00061	0.00077	0.00082
0.3	0.00155	0.00167	0.00176
0.4	0.00396	0.00390	0.00401
0.5	0.00967	0.00945	0.00981
0.6	0.02417	0.02342	0.02421
0.7	0.05986	0.05891	0.06070
0.8	0.15152	0.14980	0.15393
0.9	0.38802	0.38405	0.39367
1.0	1.00000	1.00000	1.01330

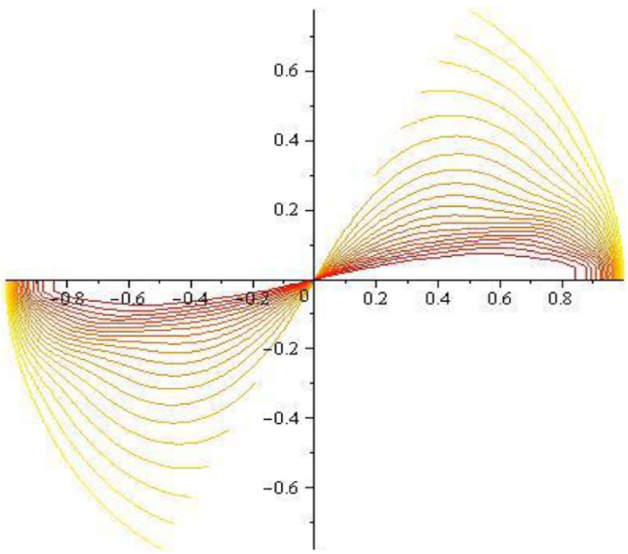

Figure 2 : Dimensionless potential for different values of ε from 0 to 1 and r from -1 to 1in cylinder coordinate

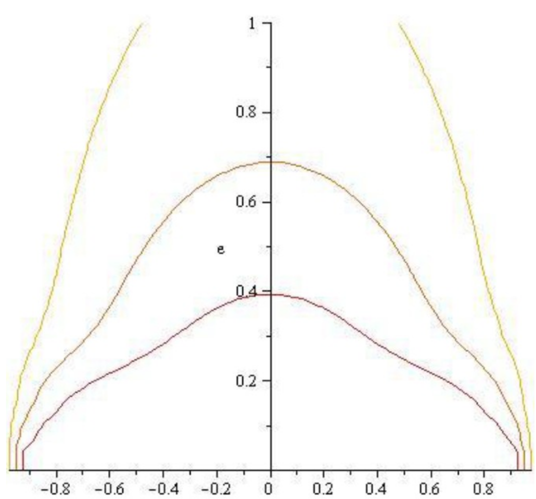

Figure 3 : Dimensionless potential amount for different values of ε from 0 to 1 and r from -1 to 1

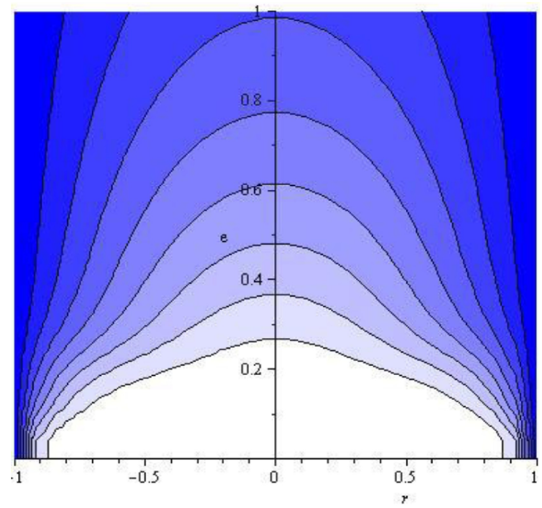

Figure 4 : Dimensionless potential amount for different values of ε from 0 to 1 and r from -1 to 1

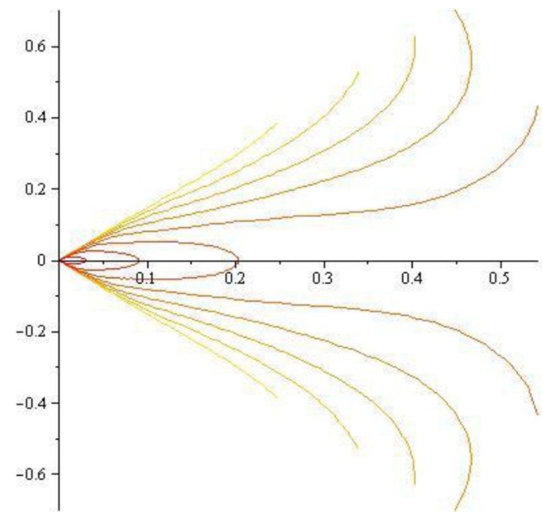

Figure 5 : Potential for different values of ε from 0 to 1 and r from -1 to 1in spherical coordinate

the relative permittivity of the solvent, the permittivity of free space and the Boltzmann's constant in different cases. Further, the temperature has its portion in increasing the potential. Moreover, the decrease in the amount of ionic strength and the elementary charge causes the potential amount to be increased.

CONCLUSION

In this work, our main concern has been to study applicability of RVIM in solving a nonlinear singular differential equation. The example presented here is the Poisson-Boltzmann equations governing electrokinetic flow inside a nano tube with small zeta potential. An approximation to the analytic solution for the range -1 to 1 was obtained by applying the RVIM Method. A comparison of the results presented in this article with the results obtained by HPM is given[10]. It suggests that the Method is accurate, reliable and easy to use. Furthermore, as it can be seen in TABLE 1, in some cases, the result that has been obtained from RVIM has more consistency with HPM solution rather than numerical ones. The nearer to the nanotube wall, the more singularity the equation has and consequently, RVIM results will have less reliability, but as it can be easily seen, over 90% of the solution field, RVIM results have more consistency than numerical results. After all, we can accept RVIM as well. As a result, after simulation, validation with other methods is mandatory in order to avoid wrong approaches. While it is obvious in paper, RVIM does not have the limitation that HPM has in finding first guess of the solution. As it has been mentioned, results in this paper are validated by other approach achieved by[12].

REFERENCES

[1] S.Kandlikar, S.Garimella, D.Li, S.Colin, M.R.King; 'Heat Transfer and Fluid Flow in Minichannels and Microchannels', Elsevier Limited, **(2006)**.

[2] B.J.Kirby; 'Micro and Nanoscale Fluid Mechanics: Transport in Microfluidic Devices', Chapter 6: Electroosmosis, Cambridge University Press, **(2010)**.

[3] D.L.Wise, D.J.Trantolo, (Eds); 'Remediation of hazardous waste contaminated soils'.

[4] D.Burgreen, F.R.Nakache; J.Phys.Chem., **68(5)**, 1084-1091 **(1964)**.

[5] H.Oshima, T.Kondo; J.Colloids and Interfacial Sci., **135(2)**, 443-448 **(1990)**.

[6] C.L.Rice, R.Whithead; J.Phys.Chem., **69(11)**, 4017-4023 **(1965)**.

[7] W.Y.Lo, K.Chan; J.Chem.Phys., **143**, 339-353 **(1994)**.

[8] H.Keh, Y.C.Liu; J.Colloids and Interface Surfaces, **172**, 222-229 **(1995)**.

[9] M.Mostofi, D.D.Ganji, M.Gorji-Bandpy; Investing the temperature effect on velocity profile in electroosmotics driven nano-channel, Proc. of 6th Nanoscience and Nanotechnology Conf., 365 **(2010)**.

[10] M.Mostofi, D.D.Ganji, M.Gorji-Bandpy; Electrokinetic flow modeling in a porous nanochannel using curvilinear coordinates, Proc. of 6th Nanoscience and Nanotechnology Conference, **(2010)**.

[11] A.T.Conlisk, J.McFerran, Z.Zheng, D.Hansford; Anal.Chem., **74(9)**, 2139-2150 **(2002)**.

[12] M.Mostofi, D.D.Ganji, M.Gorji-Bandpy; Int.Rev. Model.Sim., **3(2)**, **(2010)**.

[13] R.F.Probstein; 'Physicochemical Hydrodynamics: An Introduction', 2nd Edition, **(2003)**.

[14] E.Hesameddini, H.Latifizadeh; Int.J.Nonlinear Sci.Numer.Simul., **10**, 1377-1382 **(2009)**.

[15] A.A.Imani, D.D.Ganji, Houman B.Rokni, H.Latifizadeh, Esmail Hesameddini, M.Hadi Rafiee; Applied Mathematical Modelling, **36**, 1550-1557 **(2012)**.