Modification of Hindrance Factor due to the Presence of Charged Surface Heterogeneity

Tariq Mahbub
Dept. of Textile Engineering, Daffodil International University, Dhaka, Bangladesh

Abstract—Presence of wall at the vicinity of a moving particle through a flowing or stationary fluid hindered the motion of the particle by implying more drag on it. Presence of charge on the particle alone or on both the wall and particle hinders the motion more due to electrokinetic effect like relaxation and EDL overlap. Presence of charged surface heterogeneity make the scenario worse. A 3D finite element model consisting of Navier-Stokes, Poisson and Nernst-Planck equation has been developed to study the effect of charged surface heterogeneity on the hindrance factor for a charged particle moving along the centerline of a cylindrical channel. It has been found out that presence of charge on the particle increase hindrance factor throughout the whole channel but presence of surface heterogeneity increase the factor at its vicinity only. Effect of solution concentration and separation gap between particle and flagellum are also investigated.

Keywords—Debye length, Drag force, Hindrance factor, Relaxation, Surface heterogeneity

I. INTRODUCTION

With the advent of different miniaturization technologies micro and nanofluidic devices and the associated processes are becoming more and more key point of focus day by day. All these devices deal with tiny amount of fluid flowing through micro and nanochannels and involve different process like porous media flow, membrane filtration, electroosmosis, chromatography where motion of suspended particle plays a critical role [1-4].

Colloidal motion in water was first reported by Robert Brown nearly two hundred years ago while the effect of wall on the drag experienced by colloidal particle moving in an infinitely long cylinder through stationary fluid was investigated by Ladenburg nearly hundred years ago [5]. Since then numerous theoretical and experimental studies have been performed to elucidate this hindered transport phenomena [6-10]. The first exact solution of hindrance factor was first presented by Haberman and Shayer for a particle moving in a stationary fluid and Poiseuille flow in terms of infinite set of linear algebraic equations [9]. Their study was limited for particle to channel radius ratio, \( \lambda <0.8 \). Later single perturbation method was applied to calculate hindrance factor for a range of \( 0 \leq \lambda \leq 1 \) [11].

Different experimental study also supported these values [12-13]. Several numerical study are also performed to calculate hindrance factor numerically and more accurately. Bowen and Sharif [14], Feng and Michaelides [15], Higdon and Muldoweney [16] contributed in this discipline highly. Till then all the model used some assumptions like infinitely long channel and uniform cross section, uncharged particle. But finding infinitely long is nearly impossible in practical cases. Quddus et.al[17] investigate this issue and used Arbitrary Lagrangian Eulerian method to calculate hindrance factor in a finite length channel. Recently Deen studied the effect of charge on pore and particle on osmotic refection coefficient [18], intrapore diffusivity [19] and sieving coefficient and lag factor [20]. Despite nearly reaching its saturation effect of charge on particle and surface heterogeneity is yet to be explored more due to various biological vessel has charged surface heterogeneity and charge particle moving through it.

A finite element model has been developed to study the effect of flagella like charged surface heterogeneity on the hindrance factor also called drag factor for a charged particle moving through a finite size cylindrical channel. Centerline approximation is been considered and simplification is done by considering a rigid paraboloid shape flagellum. In this paper hindrance factor \( (K_h) \) is reported, that is particle is assumed to be hold stationary and fluid is considered moving over it. Coupled Navier-Stokes, Poisson and Nernst-Planck equation allows this model to deal with electric double layer (EDL) of any thickness. It should be mentioned EDL forms around any charged surface immersed in an electrolyte solution. When fluid flows over the surface the EDL gets distorted and give rise to a local electric field which is known as relaxation effect. When two double layer overlap a complex ion distribution is seen at the overlapped zone. Using Poisson and Nernst-Planck equation make it possible to track the complex ion distribution during relaxation and EDL overlap. The drag force is calculated by integrating hydrodynamic stress and Maxwell stress over the surface of the particle. Then the total drag was divided by stokes drag to calculate the hindrance factor.
The flow field inside the channel is governed by Navier-Stokes equation coupled with continuity equation,

\[
\rho \left( \mathbf{u} \cdot \nabla \rho \right) = -\nabla p + \mu \nabla^2 \mathbf{u} - \rho_f \nabla \psi \\
\nabla \cdot \mathbf{u} = 0
\]

Where \( \rho \) is the fluid density, \( \mathbf{u} = (u, v, w) \) is the fluid velocity vector with \( u \) and \( v \) being the radial and axial velocity components, respectively, \( \mu \) is the viscosity of the fluid, \( p \) is the pressure, \( \epsilon \) is the dielectric permittivity, \( E \) is electric field.

### II. THEORETICAL DESCRIPTION

A cylindrical channel of length \( L \) and radius \( b \) is conceived as the problem geometry. A spherical particle of radius \( a \), is considered to travel through the centerline inside the channel. A paraboloid shaped object of length \( L_f \) representing flagellum shaped surface heterogeneity is protruded in \( z \) direction from the cylinder wall as in Fig 1. Fig 2 shows the microscopic view of the geometry. The cylinder terminates in two large reservoir to eliminate any kind of end effect. An aqueous solution of varying concentration is supposed to flow through the channel from left reservoir to right one by the application of pressure.

**Fig 1: Model geometry**

**Fig 2: Microscopic view of problem geometry**

Putting all the scaled parameters in the governing equations the equations becomes,
\[ \nabla^* = \frac{h}{b} \alpha, \beta = \frac{h}{b}, \kappa b = \kappa b, u^* = \frac{u}{(\varepsilon b)(K_s T_e z_e)} \]

\[ p^* = p^* \left( \frac{b^2}{e} \right) \left( \frac{z_e}{K_s T_e} \right)^2, \rho^* = \left( \frac{e}{\mu} \right) \left( \frac{K_s T_e}{z_e} \right)^2, n_{p, e} = \frac{n_{p, e}}{n_e} \]

\[ \psi^* = \psi \left( \frac{z e}{K_s T_e} \right), E^* = E \left( \frac{z e b}{K_s T_e} \right), q^* = q \left( \frac{z e b}{e K_s T_e} \right), \]

\[ D'_{p, e} = D'_{p, e} \left( \frac{\mu}{e} \right) \left( \frac{z e}{K_s T_e} \right)^2, F' = \frac{F_b}{e} \left( \frac{z e}{K_s T_e} \right) \]

Navier-Stokes equation:

\[ \rho^* \left( u^* \cdot \nabla^* u^* \right) = -\nabla^* p^* + \nabla^* \cdot \rho^* \left( \frac{1}{2} (k b)^2 \left( n_e^* - n_e^* \right) E^* \right) \]

Poisson equation:

\[ \nabla^* \psi^* = \frac{1}{2} (k b)^2 \left( n_e^* - n_e^* \right) \]

Nernst-Planck equation:

\[ \nabla^* \left( n_{p, e}^* u^* - D'_{p, e} \nabla^* n_{p, e}^* - D'_{p, e} \nabla^* \psi^* \right) = 0 \]

The channel wall is assumed to be impermeable for the ions. Velocity at channel wall for solution is considered to be zero and zero charged on the channel wall is considered. For flagellum and spherical particle no slip condition, insulated surface and negative constant surface charge is assigned. At reservoir inlet a constant velocity is applied, zero surface potential is assigned as the reference potential and bulk concentration is conceived. At reservoir outlet zero pressure, zero surface charge and bulk concentration is assigned. At the reservoir wall, slip condition, insulation and zero surface charged is conceived.

A commercial finite element solver has been used to solve the set of differential equation along with given boundary conditions. Two different types of elements were employed to discretize the computational domain, Triangular element at the wall and Tetrahedral element inside the channel and reservoir. Fine meshes were used on the particle and flagellum surface to capture the sharp change of potential in EDL and ion distribution. Relatively coarse meshes were used in reservoir region. Mesh sensitivity analysis was carried out and approximately 110,000 elements were decided upon to obtain the result.

III. RESULTS AND DISCUSSION

A. Model validation:

Though numerous literature works are found on hindrance factor \((K_2)\) for uncharged particle of different size and shape, a little is available for charged particle. To ensure the applicability of the current computational model namely NS-3D model it is validated using both the result of uncharged particle [11, 16, 17] and charged particle [19] in Fig: 3 and 4 respectively. For charged particle excess drag is calculated by subtracting the hindrance factor calculated for an uncharged particle from the hindrance factor calculated for charged particle. Both the figure shows the accuracy of the model.

B. Effect of presence of charged flagellum:

Flagellum effects the hindrance factor in two different manners. Firstly flagellum even if uncharged will increase the hindrance factor due to the hydrodynamic effect. At the vicinity of flagellum fluid velocity will increase to keep a constant flow rate throughout the channel eventually rising the drag force on the stationary particle resulting the increase in hindrance factor.

![Fig 3: Darg factor \((K_2)\) reported by various authors and conformance of present model](image)

![Fig 4: Validation of excess drag for different size ratio](image)
Secondly, when the flagellum is considered to be charged, it will interact with charged particle via electrostatic repulsion, relaxation and EDL overlap. This will modify the hindrance factor to some extent. The effect of charged and uncharged flagellum on hindrance factor is shown in Fig 5. The plot for uncharged particle only in Fig 5 clearly shows that hindrance factor remains constant throughout the channel if there is no flagellum. As soon as there is a flagellum inside the channel at the vicinity of it, $K_2$ increases. For a charged particle and uncharged flagellum $K_2$ is higher for every position inside the channel. Relaxation results this increment. Relaxation causes a local electric field in the flow direction which produces some electrical drag, which increases the total drag resulting in an increase in drag factor. How the electrical drag contributes to the total drag force is shown in Fig:6.

It is also evident from Fig 5 that for charged particle and flagellum the hindrance factor at flagellum downstream is slightly higher than flagellum upstream. Distorted EDL overlap at flagellum downstream is the reason behind it. Distorted EDL causes more concentration gradient across the particle resulting in higher local electric field and electrical drag. The increment of electrical drag is also visible in Fig 6.

**Fig 5: Hindrance factor for different charged condition on particle and flagellum at different axial distance between particle and flagellum, $u^*=0.45$, $\psi^*=-1$, $\lambda=0.475$**

**Fig 6: Drag force on particle at different axial distance between particle and flagellum, $u^*=0.45$, $\psi^*=-1$, $\lambda=0.475$**

It clearly shows the contribution caused by the electrical drag to the total drag force felt by the stationary particle.

**C. Effect of Concentration:**

Solution concentration plays a critical role in determining the hindrance factor for a charged particle moving in an electrolyte solution. Fig 7 shows the variation of hindrance factor for different concentration for three different cases like uncharged particle and flagellum, charged particle and uncharged flagellum and charged particle and flagellum. For uncharged particle and flagellum solution concentration has no effect on hindrance factor as there is no EDL to form around the particle. For charged particle and uncharged flagellum the hindrance factor increases with concentration i.e. value of $\kappa b$. It increases more when both the flagellum and particle are charged. With the increase of concentration there exist more ion in EDL resulting in thinner EDL (larger $\kappa b$) but more concentration gradient across the particle. The local electrical field becomes stronger providing more electrical drag force. Concentration also has effect on the fluid velocity via the electrical body force term available in Navier-Stokes equation. But that contribution is negligible.

**Fig 7: Variation of Hindrance factor/Drag factor at different solution concentration, $\kappa b=0.1,1,5$, $u^*=0.45$, $\psi^*=-1$, $\lambda=0.475$**

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At lower concentration (low \( \kappa_b \)) the thickness of EDL is high enough to cover nearly the whole channel.

Another thing is that for the same size ratio with the increase of \( \kappa_b \) drag factor increases. But the increment is visible at higher size ratio. At higher \( \lambda \) the separation gap between the particle and flagellum decreases which facilitates more EDL overlap. This seems to be the reason behind it. The excess drag caused by the presence of charged flagellum at different \( \kappa_b \) is plotted in Fig 10. Excess drag is calculated by subtracting the drag factor for an uncharged particle in an uncharged cylindrical channel form the drag produced on a charged particle confined in a cylindrical channel containing charged flagellum. Here excess drag produced increases with the increase of both size ration and concentration.

IV. Conclusion

Presence of charge on the particle and charged surface heterogeneity have a great effect on the hindrance factor/Drag factor for the particle. So particle will experience more drag during flow if any or both of these remain present. This will eventually slow down the particle and for certain charge and surface heterogeneity particle motion might stop. This study can be used as the groundwork for studying blood flow in disease like Atherosclerosis, clotting and sedimentation in micro and nanochannel etc.

D. Effect of separation gap:

Drag factor for different size ratio at different solution concentration (\( \kappa_b \)) is plotted in Fig 9. The bar chart clearly shows that with the increase of \( \lambda \), drag factor increases for every \( \kappa_b \). This means the higher the particle size the higher will be the drag factor.


