A Study of the Effect of Pore Geometry on the Rejection of Nano Particles from Porous Membranes

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ABSTRACT. The study of particle motion in porous membranes requires an understanding of the impact of fluid characteristics and membrane geometrical properties on motion. The complexity of such media demands a detailed examination of the effect of membrane structure which has not been previously investigated. In this study, the motion of spherical and non-spherical particles in pore channels were modeled and the impact of pore entrance and pore bends were analyzed. A finite element method was employed to evaluate the hydrodynamic forces on particle boundaries using the Navier-Stokes equation. Steric exclusion and the rotational forces for non-spherical particle were included in the models.

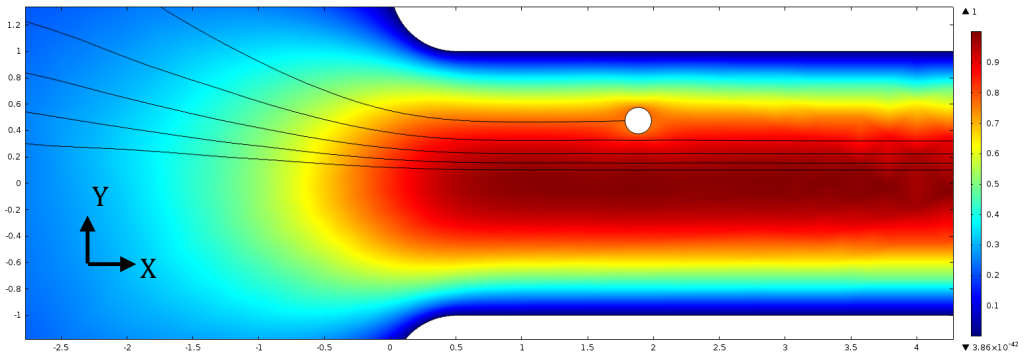


Figure 1: Particle trajectories for different initial positions in the reservoir at $X = -5$ and $Y = 5$ to 1

Several representative results are presented here. The position of a particle was tracked as it traveled from a reservoir into a pore (Figure 1). The results including the 2-D

components of velocity, drag force and position were collected and used to statistically analyze the hydrodynamic effect of the pore (Figure 2). The results indicated that the particles are concentrated near the pore centerline and do sample all the available positions inside the pore unlike the assumption used in previous studies where the particles were expected to equally sample all the sterically allowed positions based on the Boltzmann expression.

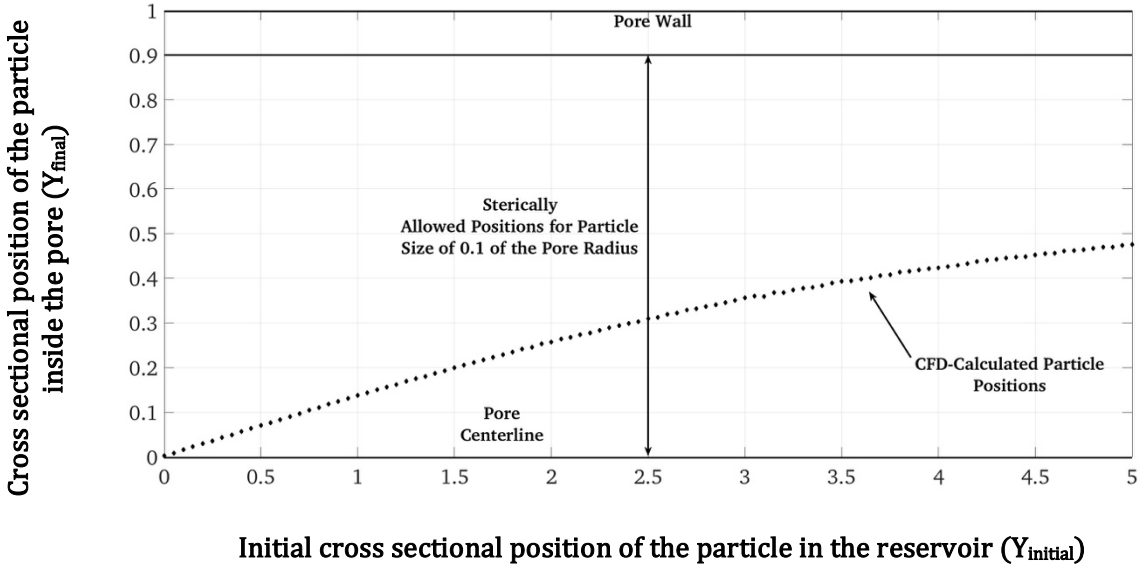


Figure 2: Cross sectional position of a particle in a pore as a function of its initial position in the Reservoir. $Y_{final}=0$* represents the centerline of the pore. The radius of the pore was assumed to be at $Y_{final}=1$*.

*** A non-dimensional scale was used for any position on the graph based on pore radius.**

The effective entrance length is defined as the distance from the pore entrance where the particle accelerates as it reaches its steady velocity. Understanding the impact of different parameters such as flow velocity, geometry of the pore entrance, etc. on this length is of great importance in determining the steady position of a particle inside a pore. The particle cross sectional position is required when evaluating the rejection coefficient of a particle in a certain pore structure.

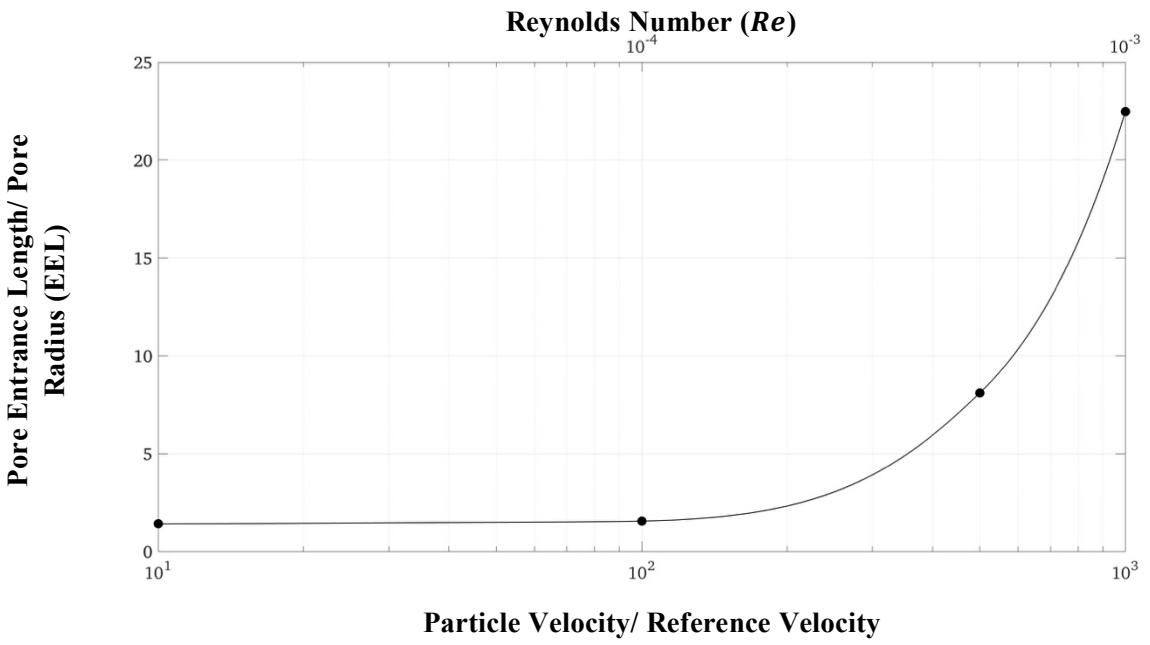


Figure 3: Effect of particle velocity on the dimensionless pore entrance length. These results span from Re = 10^{-6} to 10^{-3}. Calculations were performed for a particle with size 10% of the pore size ($\lambda = 0.1$).

The results also showed that the flow velocity has the strongest effect among all the geometrical and flow parameters on the effective entrance length where it increased exponentially with increasing the velocity (Figure 3). In Addition, Particles may not achieve a steady velocity for pores with length of less than calculated EEL for a specific Reynolds number (e.g. particles in a pore with length of 10× pore radius reach steady velocity only in Reynolds number of less than 5×10^{-4}).

This on-going project will provide a better perspective of the rejection characteristics of complex porous structures compared to previous calculations on the simple geometries (straight cylinder or channel) using the mentioned assumption for position of a particle inside a pore. This work will continue by investigating the effect of bends in pores which can greatly impact the position of the particle.