ABSTRACT

Nano-rods transportation upstream in an elliptical channel was simulated with a 2-D model. The results of the model were then compared with results obtained by a one dimensional biased walk. Through simulations we observe the interaction between the surfaces of an elliptical channel and migration of rods against flow. The Concentration profiles of nanorods upstream migration resemble a biased random walk, with an exponential run-time distribution.

INTRODUCTION

Rods exhibit micro-swimmer characteristics capable of upstream transportation. The Elliptical Dynamics Simulator (E.D.S) is focused on rod's contamination inside an elliptical channel.

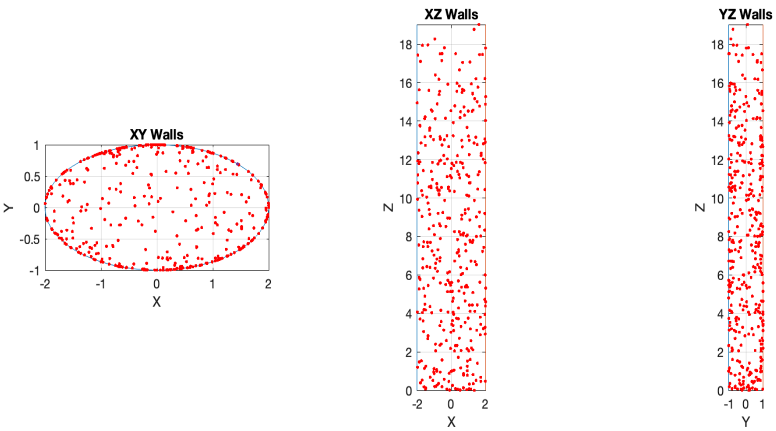

Figure 1, is the display at the end of a simulation produced by E.D.S. The 3-D channel is represented by two 2-D channels. One channel demonstrates the xz-wall and the other the yz-wall. The Ellipse shows the cross section of the elliptical channel, which allows us to see the concentrations of rods along the surfaces of the channel in the xy-plane[1]. Below we demonstrate the concentration profiles of the 1-D random walk channel and the E.D.S.

RESEARCH

Concentration profiles along the z-axis of E.D.S are shown as a snapshot at time (t), where we can see the positions and quantities of swimmers along the channel. Fig 02 depicts the quantity of swimmers (y-axis) that are currently at the z-position (x-axis). As the time moves forward we see the horizontal portion of the profile increase in its length, moving the starting point of where the concentration drops off, further up in the channel. This indicates that the density of rods at higher positions increase over time.

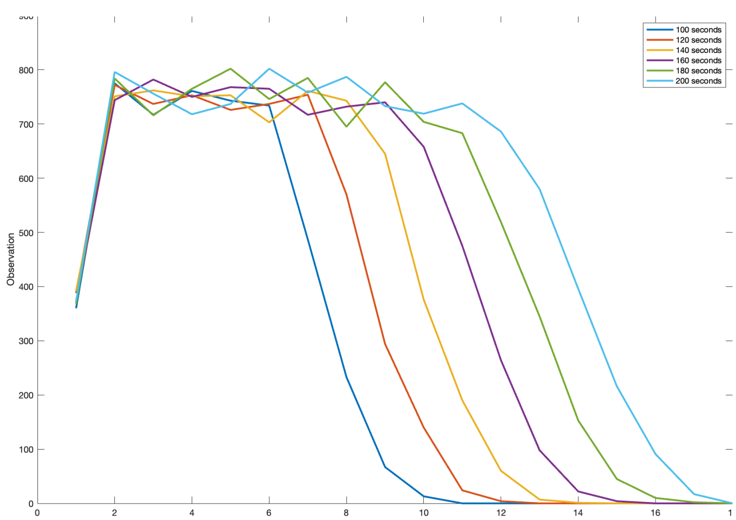

Fig 02 Concentration profiles taken at different times, where rods are entering at a constant rate.

[1]The perspective is analgous to looking inside a tube.

The concentration profiles which resemble the exponential distribution of run-times depicts rods upstream transportation, with a greater quantity of rods traveling greater distances than if it resembled a power-law runtime distribution. Figure 03, compares a contamination profile produced by a random walk with an exponential runtime distribution and a contamination profile produced by E.D.S. Clearly showing the similarities between the two[2]. Being able to simulate model upstream transportation by a one dimensional random walk greatly decreases the amount of computation when compared with the E.D.S simulation.

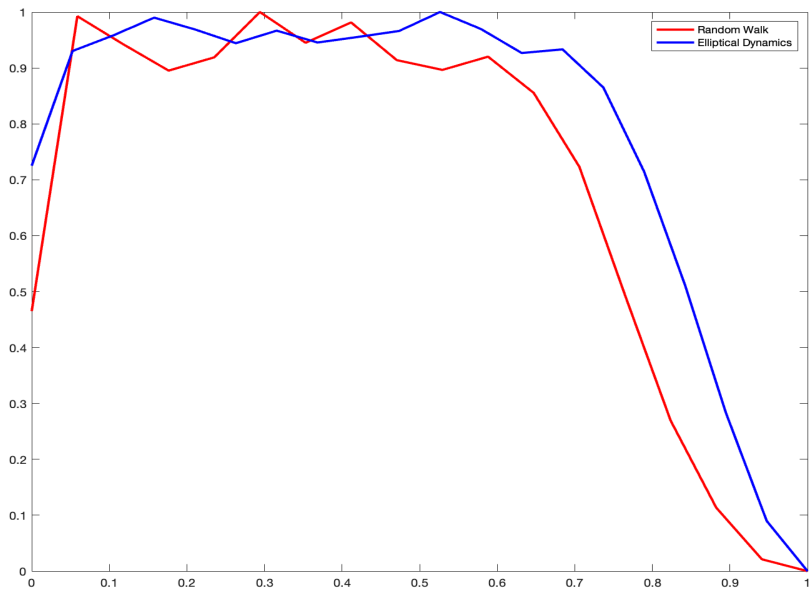

fig 03 comparison of a contamination profile generated by a one dimensional random walk and one generated through E.D.S.

DISCUSSION

Our results differ from results demonstrated in the Super-Contamination article (1). Where the results of a rectangular channel were reported to resemble a biased random walk with a power law run-time distribution(1). This is believed to be due to the differing geometry of the channels. During simulation certain observations were made, however due to the constraints of our simulator and time these observations remain without evidence to further support. We leave these observations open for further research.

Euler's numerical method was used to approximate the positions of our rods, and no other numerical methods were implemented to incorporate in the simulation. Since all numeric methods contain some degree of error, the question arises if there are better methods, of higher accuracy, to approximate the rods positions.

The one dimensional biased random walk was implemented to model both exponential and power-law run distributions. During simulation we found that even when we maintain an exponential restriction on the runtime distribution, that when the distance rods are advected downstream is large enough, we are able to force biased random walk to resemble a power-law distribution. Determining the main factors that factor into the one dimensional walks distribution profiles, may lead to further insights on upstream transportation.

[2] The data is normalized with a min max normalization for comparison.

Lastly, Within our simulation we are able to see the concentrations of rods along the curves of the channel, however areas of low curvature appear to be favored by the rods, during upstream transport, as seen in figure 04. What causes the rods' attraction to areas of low curvature as opposed to areas of high curvatures?

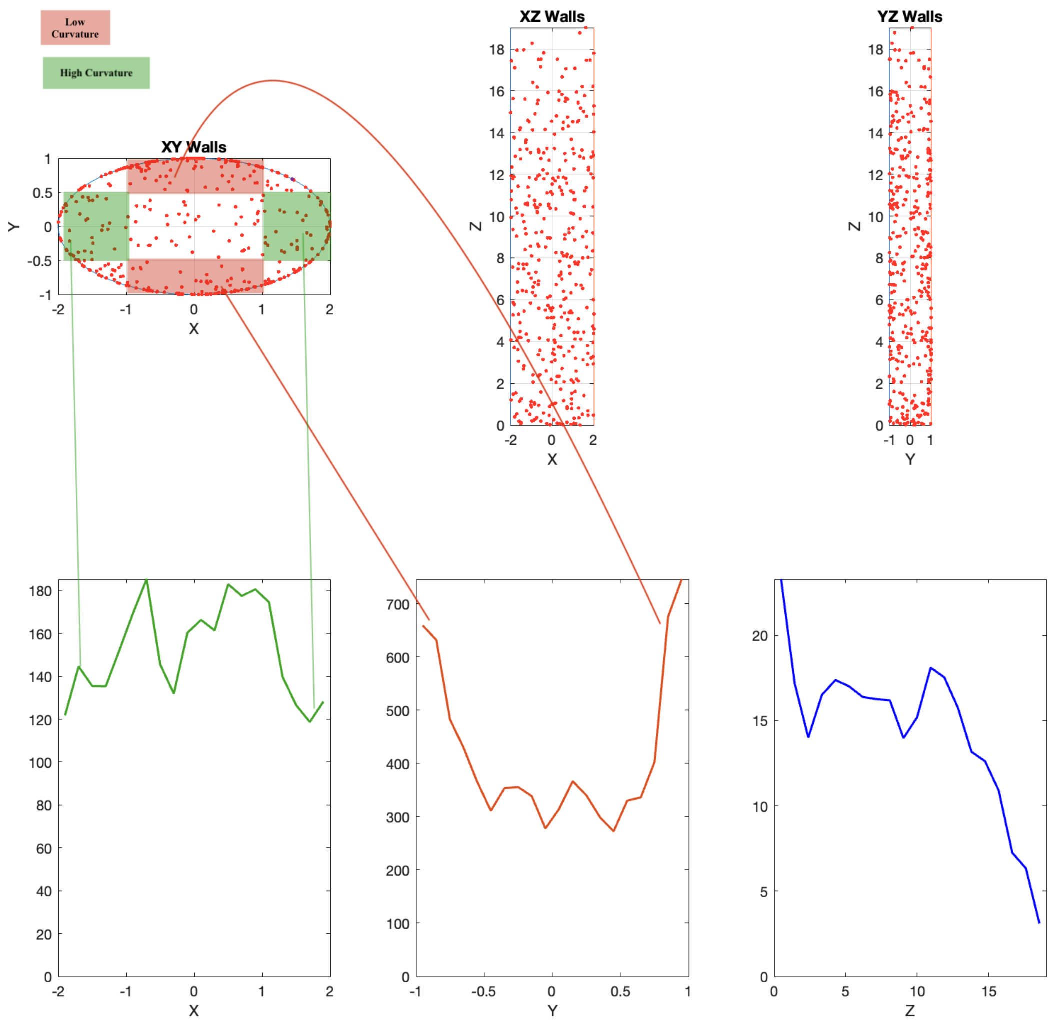

Fig 04 annotated image of the E.D.S, demonstrating the concentration of rods on low and high curvature point of the channel.

METHODS

The E.D.S, applies Euler's method to approximate the positions of the rods.
(F_{rate}) is the flow rate of the simulation, (r_a) radius of ellipse in the x-direction, and (r_b) radius of ellipse in the y-direction. Let (α) denote a randomly generated value [0,1].

$$0 \leq \theta \leq 2\pi, \quad 0 \leq \phi \leq \frac{\pi}{2}$$

$$x_n = cos(\theta_{n-1})sin(\phi_{n-1}), \qquad y_n = sin(\theta_{n-1})sin(\phi_{n-1})$$

$$z_n = cos(\phi_{n-1}) + F_{rate}\left[\left(\frac{x^2_{n-1}}{r^2_a} + \frac{y^2_{n-1}}{r^2_b}\right) - 1\right]$$

$$\theta_n = F_{rate}(- sin^2(\theta_{n-1})cos(\phi_{n-1})\frac{2x_{n-1}}{r^2_a} + \sin(\phi_{n-1})\frac{2y_{n-1}}{r_b^2}$$

The One-Dimensional Biased walk has a fixed downstream displacement time, and applies the metropolis algorithm to alter the directions of swimming and randomly generates the distances traveled upstream.

REFERENCE

(1)

Nuris Figueroa-Morales
et al. ,E. coli “super-contaminates” narrow ducts fostered by broad run-time distribution.*Sci. Adv.***6**,eaay0155(2020).DOI:10.1126/sciadv.aay0155