2D and 3D Stochastic Modeling of Membrane Fouling

Paulo Paz, Mehtab Sidhu, Catherine Sousa, Lou Kondic

New Jersey Institute of Technology, Department of Mathematical Sciences

Abstract

Membranes are used in nature and are now being used commonly in industrial processes to filter out undesired solute from suspensions, etc. These membranes typically lose efficiency over a period of time because of plugging, degradation, and is generally referred to as membrane fouling. The focus of our study is to develop specifications for the optimal pore orientation in the membrane media that resists fouling. As part of this study, we used a mathematical model to simulate fouling including adsorption, and cake layer formation as followed by Tracey and Davis [2]. We modified the pore orientation to generate an optimum orientation at which the resistance to fouling was substantial. Afterwards, a Monte-Carlo approach was implemented to simulate the 2D and 3D particle fluid flow through the membrane and resulting statistical analysis will be presented.

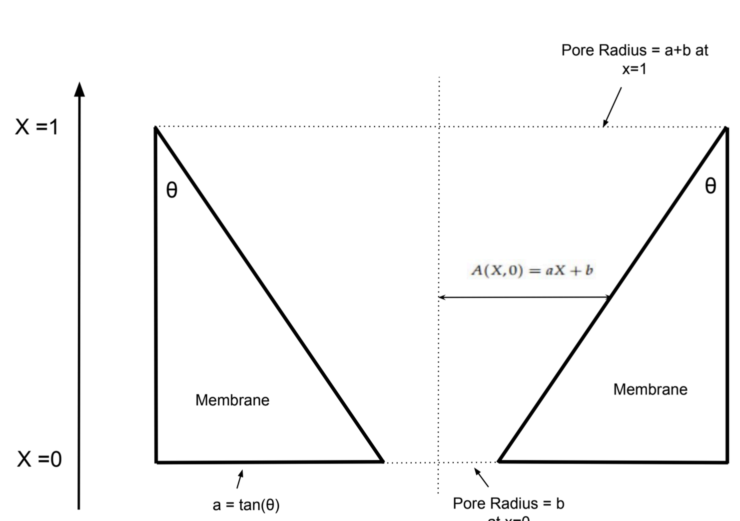
Mathematical Formulation

We are particularly interested in morphologies with pore radii that decrease linearly as you traverse the length of the membrane from the pore opening to closing. As such we refer to A(X,T) as the radius of the pore as a function of X (the vertical direction) and T time units where the number of starting particles is our measure for time. According to Darcy`s Model for flow through a porous medium [4] the local membrane resistance is proportional to $A(X,0)^{-4}$ where A(X,0)=aX+b. This implies that the average membrane resistance (after substituting u=aX+b) is given by:

$$r(t) = \int_0^1 \frac{dx}{A(X,0)^3} = \int_0^1 \frac{dx}{(aX+b)^3} = \frac{1}{a}\int_b^{a+b} \frac{du}{u^3}$$

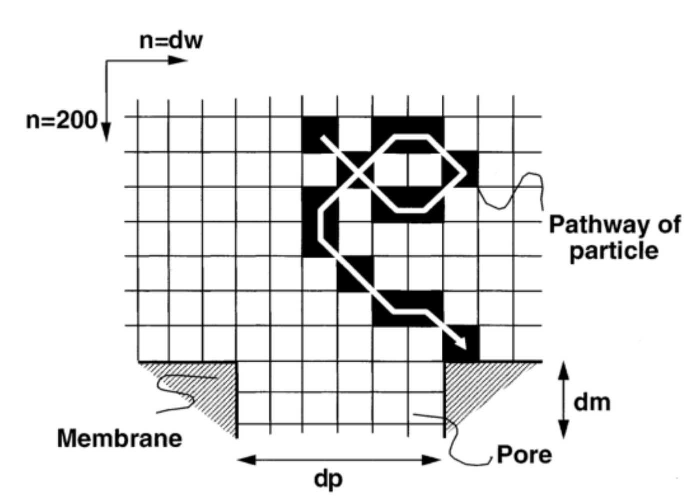
$$= \frac{1}{2a}\frac{1}{u^2}\Big|_{a+b}^{b} = \frac{1}{2}\left[\frac{a+2b}{b^2(a+b)^2}\right]$$

We were able to formulate various pairs of coefficients, a and b, for a range of angles. Using those coefficients we will alter the simulation methodology to generate different membrane profiles. This will be done by implementing the formulation of the membrane as a function of a and b. To begin we must first discretize the geometries of our simulation. The coefficients generated will form a membrane with height of 1, ranging from X = 0 to X = 1, however, for our simulation, we need to generate the membrane for a wider range of X- values.



2D Model Implementation

Our first objective was to simulate the deposition of a particle on a micro-filtration membrane, an algorithm known as diffusion limited aggregation (DLA) was used. DLA is the process of placing a stationary seed in a lattice, then releasing a mobile particle at a random location. At this point the particle performs a random walk through the lattice until it meets the stationary seed and attaches to it. Another mobile particle is then added to the lattice and the process is repeated. For our implementation, a lattice is to be initialized with a height of 200 grid points and a width of 100 grid points and membrane located at the bottom of the lattice. As the particle moves throughout the lattice it may come in contact with the membrane or other particles that have been attached to the membrane, also known as an aggregate. When the particles touch the membrane or aggregate, it remains in the position depending on an additional parameter, the sticking probability for the membrane (SPM) and the sticking probability for the aggregate (SPA). See the figure below for an illustration of the simulation lattice.



A* (ASTAR) Algorithm

To determine if a pore is clogged, our problem is reduced to a path-finding algorithm; i.e. if we're able to find a path from the top of the lattice to the bottom (through the membrane) then we can conclude that the pore is not clogged. The A (A STAR) search algorithm is a path finding algorithm that implements heuristic search to efficiently find a path with the least cost [5]. The cost of a node is denoted by*

f(n)=g(n)+h(n)f(n)=g(n)+h(n),

where g(n) is the cost from the start node to current node n, and h(n) is the heuristic estimate or estimated cost from current node n to the final node. We estimate the h value using the Chebyshev distance with

h(n)=max(|current.x - goal.x|, |current.y - goal.y|)

X,Y denote their respective X and Y positions on the lattice, and f(n) estimates the lowest total cost of any solution through node n. At each point, the node with the lowest f value is chosen for expansion, and the process repeats itself.

There are a maximum of 8 possible directions in which we can search (in 2D space: up, down, left, right, up-left, up-right, down-left down-right). Typically, this results in an exponential run time because each possible path will be fully explored in search of the optimal path. However, the heuristic algorithm like A looks at the most likely neighboring nodes that would result in a path based on the f value detailed above.*

Normal Distribution

To better examine the performance of our filter, we'd like for the particles to be forced through the membrane (using advection flow) via a normal distribution (instead of a typical uniform distribution). Suppose X N(μ,σ²) has a normal distribution and lies within the interval X∈(a,b), −∞≤a<b≤∞. Then X conditional on a<X<b has a truncated normal distribution. Its probability, f, for a≤x≤b, is given by

$$f(x;\mu,\sigma,a,b) = \frac{\phi(\frac{x-\mu}{\sigma})}{\sigma\left(\Phi(\frac{b-\mu}{\sigma}) - \Phi(\frac{a-\mu}{\sigma})\right)}$$

Using a brute-force method, we were able to conclude that σ≈0.9 and the probabilities were as follows:

0.12		0.12
0.22	0.29	0.22

Normal Distribution

0.2		0.2
0.2	0.2	0.2

Uniform Distribution

3D Model Implementation

The lattice will be set to one of 3 integers: 0 denoting an empty space, 1 denoting the membrane, and 2 denoting a particle. Considering strictly the filter (and ignoring creating the empty space above which is trivial) the dimensions of the "cube" will by [−(a+b), a+b] × [−(a+b), a+b] × [0,1] where the z-direction (height of the membrane) is given by the interval [0,1]. And the equation for our cone is:

$$x^2 + y^2 = (az + b)^2$$

Note that at z=0, the radius at the bottom of the filter is r=b, and similarly at z=1, the radius at the top of the filter is r=a+b. We'll give the z-direction some discrete values i.e $z_i = hi$ for i=0,..,N and h=1/N where N denotes the resolution of our grid. We can iterate over all z_i and fix the equation of the membrane to be: $x^2 + y^2 \geq (az_i + b)^2$

After fixing z_i, we similarly discretize the x- and y-direction using the previous relationship, setting the lattice =1 if this relationship is satisfied, otherwise setting the lattice =0. Using this logic, we can create the membrane and extend the z-direction to include the empty spaces to initialize our particle. This methodology can be seen in figure 1 and 2 below.

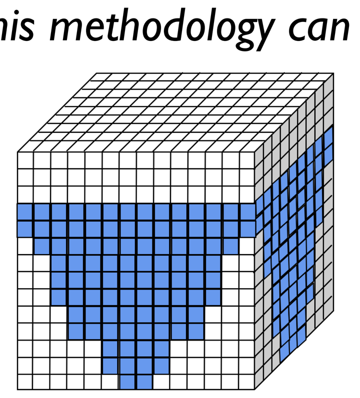


Figure 1

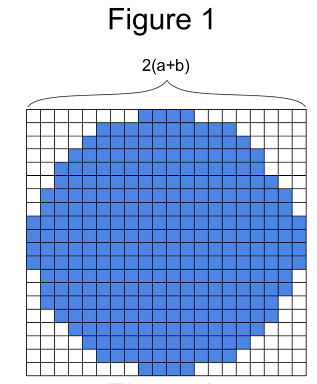


Figure 2

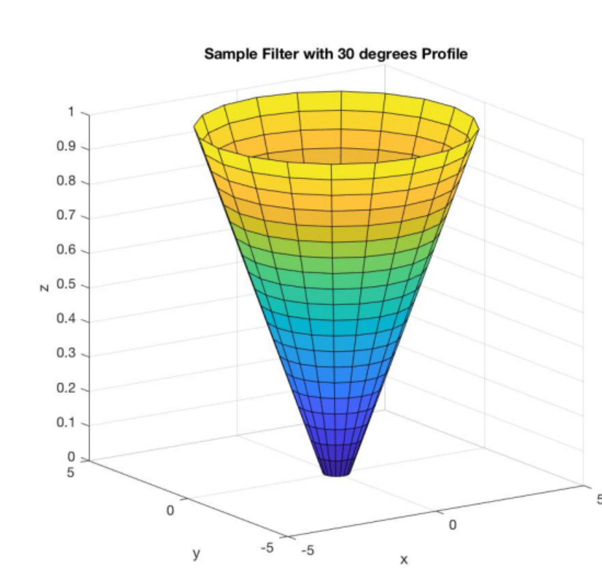


Figure represents conical cylinder

Results

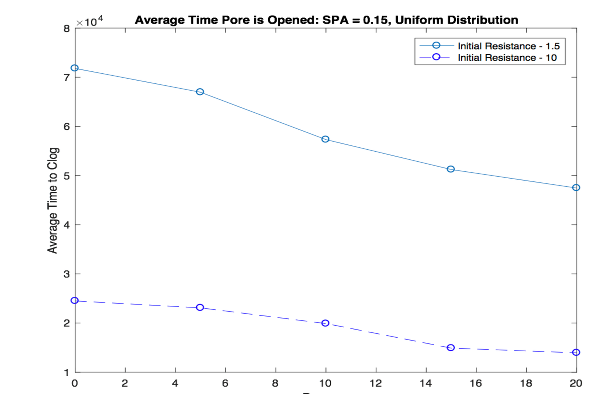


Figure 1

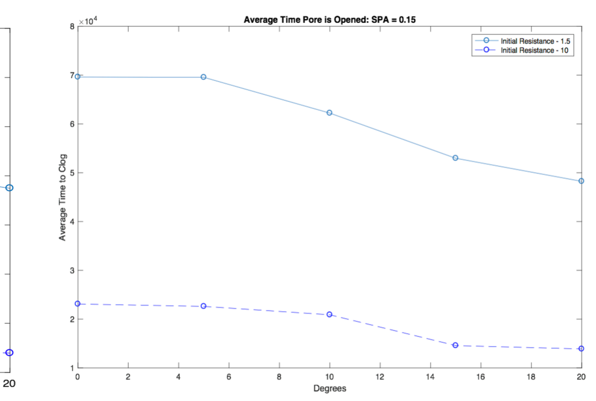


Figure 2

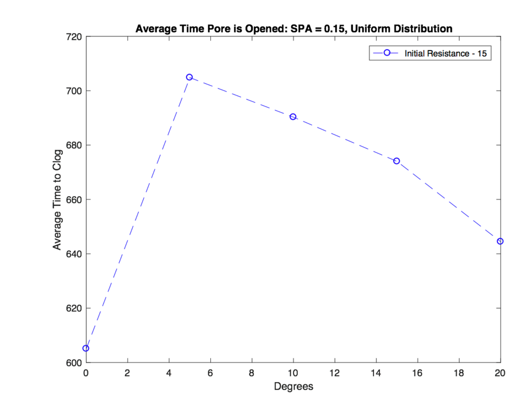


Figure 3

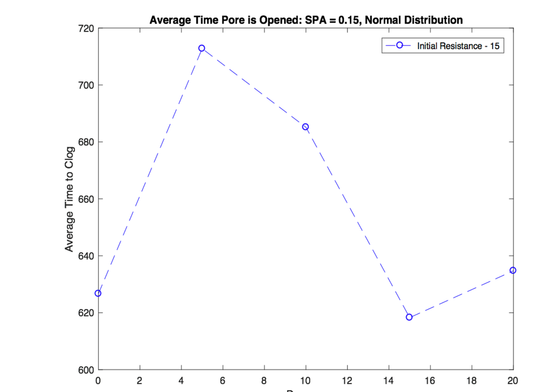


Figure 4

We performed 50 simulations for various degrees then averaged the clogging time over the 50 simulations to get an estimate of the average clogging time. From figures 1 and 2 we don't observe a global maximum, however it can be seen that the slope near the origin decreases as resistance increases which agrees with previous research. Resistance was increased once more to 15 and we successfully observed the characteristic global maximum in addition to the angle which agrees with research on the angle considered the "optimal angle" (figures 3 and 4).

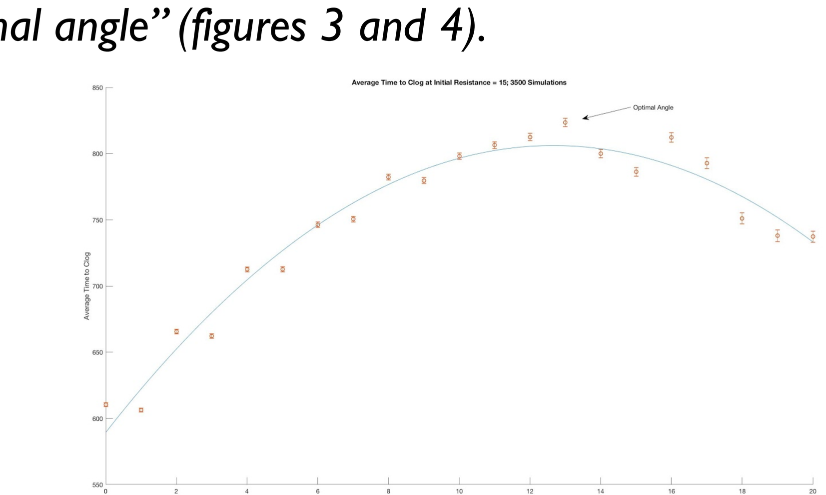


Figure 5

Significantly increasing the number of simulations run to 3500 and refining the interval of degrees to search over [0, 20], the results were plotted along with the standard error bars (figure 5). For a pore profile with initial resistance 15, we have statistically significant results to conclude that the optimal linear profile is with an inclination angle of 15 degrees.

References

[1] M Wessling, Two-dimensional stochastic modeling of membrane fouling, Separation and Purification Technology, Volume 24, Issue 3, 2001, Pages 375-387 https://doi.org/10.1016/S1383-5866(01)00138-1.

[2] E.M. Tracey, R.H. Davis, Protein fouling of track-etched polycarbonate microfiltration membranes, J.Coll. Interf. Sci. 167, 104-116 (1994).

[3] K. Nakamura, K. Matsumoto, A mathematical model of internal fouling in protein microfiltration, J.Chem. Eng. Jpn. 31, 536-544 (1999)

[4] Sanaei, P., and Cummings, L. (2017). Flow and fouling in membrane filters: Effects of membrane morphology. Journal of Fluid Mechanics, 818, 744-771. doi:10.1017/jfm.2017.102

[5] P. E. Hart, N. J. Nilsson and B. Raphael, "A Formal Basis for the Heuristic Determination of Minimum Cost Paths," in IEEE Transactions on Systems Science and Cybernetics vol. 4, no. 2, pp. 100-107, July1968. doi: 10.1109/TSSC.1968.300136