Modeling Filtering Process Using Stochastic Simulations of Monte-Carlo Type

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Abstract

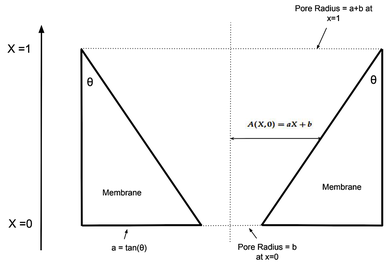
Filtration media have improved over the years to address a multitude of problems, but porous membrane filters continue to suffer efficiency losses due to fouling, which occurs even when the pores are much larger than the suspended particles via particle deposition on the pore interior walls. The focus of this research is to develop specifications for the optimal pore shape in the membrane media to maximize the filter lifetime (defined to be the time at which pores of the membrane close fully), while ensuring adequate removal of impurities. For this purpose, we have developed stochastic simulations of Monte-Carlo type to simulate fouling and to study the effect of various parameters on performance. We focus particularly on the probabilities of particles sticking to each other and to the pore walls, as well as on the influence of a cross-flow. Our model is used to investigate the performance of a membrane, modeled as multiple adjacent pores. Parameters studied include the strength of the cross-flow along with the pore size variation, both in the depth of the membrane and in the direction of the cross-flow. We use our results to draw conclusions about optimal filtration scenarios.

Mathematical Formulation

We study membrane morphologies in which the pore size decreases linearly in the depth of the membrane. For computational efficiency in our study we restrict attention to 2D membranes, in which pores are modeled as 2D channels, of width A(X,T), with X the vertical coordinate and T time. Within our Monte-Carlo framework, particles are released successively as described below; the cumulative number of particles released is our proxy for time. According to Darcy`s Law for flow through a porous medium [4] the local membrane resistance is proportional to $A(X,0)^{-3}$, where A(X, 0)=aX+b. This implies that the average initial membrane resistance is given by:

$$r(0) = \int_0^1 \frac{dx}{A(X,0)^3} = \frac{1}{2}\left[\frac{a+2b}{b^2(a+b)^2}\right]$$

Different choices of the parameters a and b allow different pore opening angles to be investigated.



Acknowledgment

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2D Model Implementation

Our first objective is to simulate the deposition of particles on a micro-filtration membrane. We use the algorithm known as diffusion limited aggregation (DLA). DLA is the process of placing a stationary seed in a lattice, then releasing a mobile particle at a random location. 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 and a width of 100, with the membrane located at the bottom of the lattice (figure 1). As each particle moves throughout the lattice it may come in contact with the membrane or other particles that have been attached to the membrane (collections of such particles are known as aggregates). When the particle reaches the membrane or aggregate, a sticking probability to the membrane (SPM) or sticking probability to the aggregate (SPA), respectively, is used to determine whether the particle will remain attached or continue to move through the lattice. To simulate the downward movement of particles through the membrane, we implemented a uniform distribution where a particle is equally likely to move in any of 5 directions, as shown in figure 2.

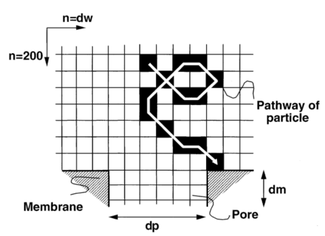


Figure 1

0.2		0.2
0.2	0.2	0.2

Figure 2: Uniform Distribution

A* (ASTAR) Algorithm

To determine if a pore is clogged, our problem is reduced to a path-finding algorithm; i.e. if we are 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 a heuristic search to efficiently find a path with the least cost [5]. The lowest total cost of any solution through any node n is denoted by*

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

where g(n) is the cost from the start node to node n, and h(n) is the heuristic estimate of cost from node n to the final node. With the goal node at location (x_1, y_1) and the current node n at location (x_2, y_2), we estimate the h value using the Chebyshev distance with

$$h(n)=\max(|x_2 - x_1|, |y_2 - y_1|)$$

At each step, the algorithm will calculate f(n) for every possible next step and will choose the node with the lowest f, and the process repeats itself.

There are a maximum of 8 possible directions in which we can search in 2D space, which would result in an exponential run time for a search algorithm, however, a heuristic algorithm like A cuts down run time by looking solely at the most likely neighboring nodes based on the f value detailed above.*

Normal Distribution

To better model a real filter membrane, we use a biased Brownian walk to impose a "flow" on the system. Suppose $X \sim N(\mu, \sigma^2)$ has a normal distribution and lies within the interval $X \in (a,b), -\infty \le a < b \le \infty$. Then X conditional on a<X<b has a truncated normal distribution. Its probability, f, for $a \le x \le b$, where a and b are the parameters used in the resistance equation previously described, is given by

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

where $\phi(\xi) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}\xi^2\right)$ is the probability distribution function of the standard normal distribution and $\Phi(x) = \frac{1}{2}\left(1 + erf(x/\sqrt{2})\right)$ is its cumulative distribution function.

Assigning values for a, b, μ, and σ gives rise to differently biased particle walks. With $a = -\frac{\pi}{2}$ $b = \frac{\pi}{2}$ and $\mu = 0$, a value of $\sigma \approx 0.9$ gives the probabilities in figure 1 below, while $\sigma \approx 0.9999$ produced the probabilities for a biased Brownian walk with a stronger tendency to move downward as shown in figure 2 below. Linearly decreasing values of σ and μ produce the cross-flow used for the 10-pore model.

0.12		0.12
0.22	0.29	0.22

Figure 1: Normal Distribution

0.000		0.000
0.049	0.902	0.049

Figure 2: Stronger Normal Distribution

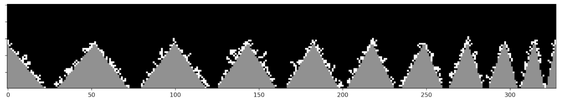
0.2		0.2
0.2	0.2	0.2

Original Uniform Distribution

We use this biased Brownian walk to determine the optimal pore profile parameters a, b that give the longest pore lifetime, for fixed initial resistance r(0).

10-Pore Model Implementation

Using the optimal pore profile from the single-pore model, 10 adjacent identical pores are generated. A second model of 10-pores is also developed with the implementation of a linearly decreasing pore size which is calculated such that the first pore on the left has the ideal membrane profile as determined by the 2D model and the pore on the far right has a width that is half that of the original, similar to that of the figure below. The performance of these two 10-pore models was studied and compared to see which performed the best.



Size of first pore (far left) to size of tenth pore (far right) follows a ratio of 2 to 1

In addition to the above alterations, a cross-flow and new biased particle walk is implemented. This is done by implementing a linearly decreasing equation to the above variables of μ and σ such that while the particle is above the pores, there exists a cross-flow from left to right that shifts as the particle moves farther down in the lattice towards the pore openings. When the particles are in the pore, a biased Brownian walk is implemented that forces the particles through the pore.

Results

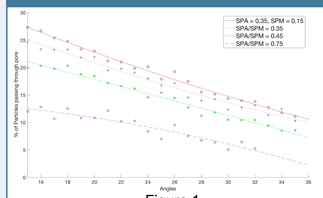


Figure 1

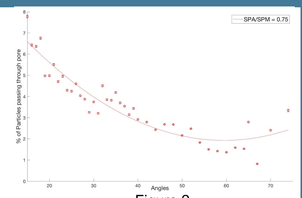


Figure 2

As seen in Figure 1 above, data collected from various combinations of sticking probabilities to the aggregate (SPA) and sticking probabilities to the membrane (SPM) with particles moving under an unbiased Brownian walk suggests that the percentage of particles escaping through the pore is minimized for SPA = SPM = 0.75. Further simulations run over a wider range of angles show that a pore angle of approximately 60 degrees performs optimally. These simulations were then run again with particles moving under a biased Brownian walk with a stronger tendency to move downwards, with results showing optimal performance for a pore angle of 40 degrees (figure 3).

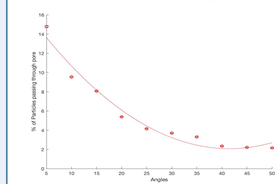


Figure 3

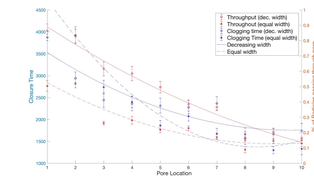


Figure 4

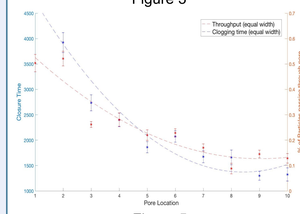


Figure 5

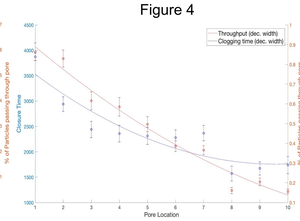


Figure 6

The arrays of identical pores in cross-flow behave differently to arrays in which pore size decreases in the cross-flow direction as can be seen in figure 4. Although the arrays of identical pores allow an average of 0.29% of particles to escape (figure 5), the individual pores in arrays in which pore size decreases in the cross-flow direction have more uniform closure times, and only allow an average of 0.47% of particles to escape (figures 6). Ideally, all 10 pores should clog simultaneously which leads to the conclusion that an optimal ratio of pore size would be above the tested 2 to 1 ratio (size of pore at location 1 to size of pore at location 10).

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