Simple Filtration Using Porous Media

Problem presented by
U. Beuscher
Gore

Participants:

S. Altrichter	J. Barton	R. Bauer
R. Booth	J. Bratz	P. Canepa
Q. Chen	J.D. Fehribach	M. Gratton
N. Greaney	W.J. Law	L. Martinez
G. Moore	A. Ortan	J. Phillips
V. Quenneville-Belair	B. Rife	L. Rossi
A. Rubio	D. Signori	S. Swaminathan
P. Vu	P. Webb	J. Zheng
Q. Zhu		

Summary Presentation given by R. Booth, 15 June 2007.
Report prepared by S. Altrichter, J. Barton, R. Bauer. R. Booth, J. Bratz, P. Canepa, J.D. Fehribach, L. Rossi, S. Swaminathan, P. Webb, J. Zheng & Q. Zhu

1 Introduction

This work is a study of the movement of particles, one at a time, through a fixed filter. Various assumptions are made about particle and pore sizes, pore selection rules and filter configurations. This report is divided into three main sections: The first studies the filter by analyzing its layers both in a qualitative sense and by computational simulations. The next studies the filter through a set of continuum models. The last consider a network model.

In the layer model a porous media is represented as a rectangular array, with each point in the array representing a single pore in the media. This divides the media into a series of layers, with the same number of pores in each layer. When a particle encounters the media it selects a pore from the first layer. If the particle diameter is greater than or equal to the width of the pore then the particle clogs that pore, and the pore is no longer available for future particles. If the particle is smaller than the pore then it passes through to the next layer and now a pore in the next layer is chosen and the process continues until either the particle leaves the media, or gets stuck in a pore.

One of the most important issues that must be determined in a layer model of a filter is the spread. The *spread* is the set of pores in the $(n+1)$-st layer that can be reached by a particle which has made it through a larger pore in the n-th layer. The two opposite extreme choices are, on the one hand, to assume that the particle can only move straight through to the pore directly below, or on the other hand, to assume that the particle can reach all pores in the next layer below. Both of these extremes seem problematic, though one might imagine a model where all pores are reachable but with decreasing probability of being reached based on the lateral distance the particle would need to move. In the layer work below, the spread is specified in each case; a specific spread rule is given in each layer subsection of this report.

The key quantity to be discussed and modelled in this work is the retention curve for a filter. A sample retention curve is shown in Figure 1. Notice that there is a plateau in the retention curve

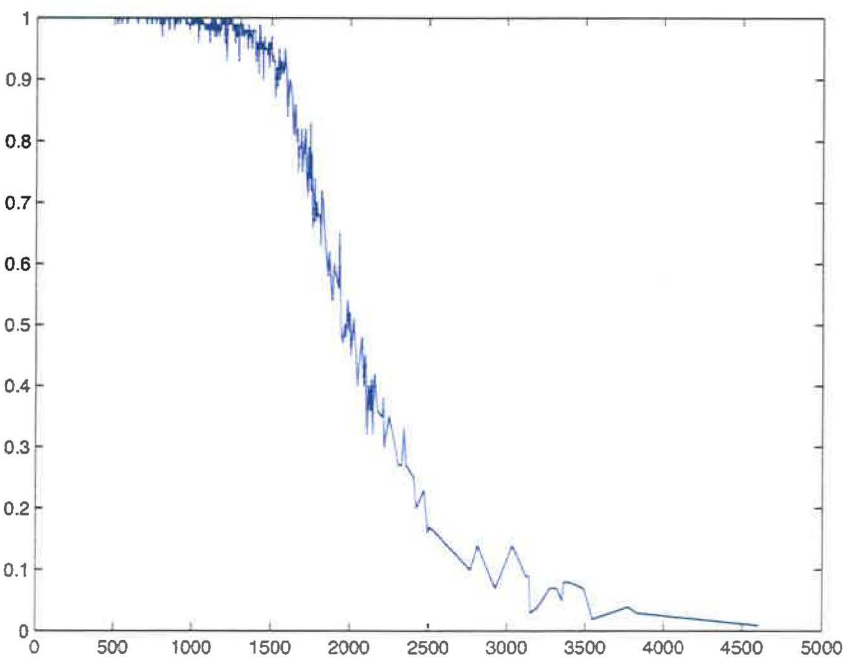

Figure 1: A sample retention curve for a typical filter. This is a plot of the probability of a particle being trapped versus the number of particles entering the filter.

for roughly the first thousand particles, followed by a dramatic drop off after roughly 1400 particles. During the plateau period, almost all of the particles are retained by the filter, Throughout this report, filtration time will be measured in number of particles filtered, *i.e.*, no attempt will be made to consider filters whose performance depends on the rate at which particles are filtered.

The second portion of this report considers several continuum models of filtration. The first continuum model assumes that all the pores in the filter are of one of two sizes (small and large), and all the particles are of a size in between these two pore sizes. The probability that a particle becomes trapped is assumed to be independent of the fraction of the pores that are blocked. This is a simplistic approach, but it provides basic incites into the problem. In a second continuum model, the probability that a particle becomes trapped is taken to be inversely proportional to the sum of the number of large and small pores open after the k-th particle has entered the filter. Finally the model is generalized to allow two particle sizes and three filter sizes.

All of the continuum models, however, still implicitly assume the filter to consist of a number of layers with pores of specified sizes. The last section considers a network model where the filter is not assumed to have layers. Nonetheless, the noetwork model since leads to a Lambert W function as the key to the solution of the crucial ODE.

There has been previous work done that relates to this problem. Datta & Redner [2] considered clogging in depth filtration. Three cases are considered, one in which the pore size is larger than the particle, one where the pore size is smaller than the particle, and one case in which there are multiple particles that clog one pore. In the third case, on the boundary between the first two cases, it takes longer for the pores to be clogged giving a delayed retention rate.

In Lee & Koplik [4], two models are considered. The first model is a simple model without blocking, meaning that there are small and large pores, and once the smaller pores are blocked with particles, other particles can continue to move through that pore. This model was fully analyzed, but is not realistic and the behavior is different from the more complicated second type of model, which is a model with blocking. In this model they found that a steady state occurs when no additional particles are trapped. The behavior of the steady state depends on the fraction of trapping pores, or "blocking probability," which is defined as p. If p is less than the threshold value then a new particle entering the media will pass through the media, and if p is greater than the threshold value then all paths are blocked in the media allowing no particles to pass through.

In Hwang & Redner [3], infiltration is discussed where the pores are much greater in size than the particles. The pores are lined with defender sites that trap particles. Once all the defender sites are filled, all particles can freely move through the pores. This article gave a similar retention result to the original problem, and this prediction agreed with experimental results.

Roussel, Nguyen & Coussot [7] take a probabilistic approach and discuss the variations of residue as a function of a variable D. The residue is the ratio of the mass of the particles remaining in the media to the initial mass of particles, and D is the ratio of the pore diameter to the particle diameter. The residue curve looks very similar to the retention curve in the original problem. This paper is also backed by experimental data and considers multiple particles moving through the media.

Other articles take a different approach to the porous media problem. Redner & Datta [5] as well as Chang & Chan[1] use models that describe a situation where the filter gets to a point of complete clogging where no particles pass through. Rege & Fogler [6] discuss a network model that considers the fluid velocity as well as the ratio of particle size to pore size. Shin [8] looks at flow through porous media using numerical methods such as the finite element method. The filter which was used in this case had a periodic lattice structure. The results were qualitatively similar for three different Reynolds numbers.

There are a small number of parameters and indices which will be used throughout this report:

$$\begin{array}{rcl} k & : & \text{particle index} \\ K & : & \text{total number of particles} \\ n & : & \text{layer index} \\ N & : & \text{total number of layers in the filter} \\ m_n & : & \text{pore index for the } n\text{-th layer} \\ M & : & \text{number of pores per layer layer} \end{array} \tag{1}$$

2 A Layered Description

This section of the report discusses our work on layer models, i.e., discrete models that consider how specific particles move through specific pores in specific layers. All models discussed here are

```
### ####     ##     #### ####     ##     #### ###### ####     #### ###
#     ##     #### ###### ####     #### ####     #### ####     ##     #
#     ##     ##     ##     #### ####     ##     ##     ##     #### ###
### ###### ####     ##     #### ###### ###### ###### ####     ##     #
### ###### ###### ####     #### ####     ##     #### ###### ###### ###
#     #### ###### ###### ####     #### ####     ##     ##     ##     #
#     ##     ##     ##     #### ####     ##     #### ####     #### ###
#     ##     ##     ##     #### ####     ##     ##     ##     #### ###
### ###### ####     #### ####     #### ###### ###### ####     ##     #
#     ##     #### ###### ###### ###### ####     ##     #### ###### ###
```

Figure 2: A portion of a filter cross section (or two-dimensional filter). Hash (or number) signs represent the filter walls, and blank spaces, the pores themselves. In this diagram, $N = 10$, $M = 10$ and there is a random distribution of two pore sizes (large and small).

two dimensional. In these models the most important issue is the *selection rule* or *spread*: the rule that decides which pore in the $n+1$-st layer a particle making it through the n-th layer goes to. The possibilities discussed below range from every open pore in the $n+1$-st layer being equally available to the particle to only the two or three pores in the $n+1$-st layer nearest the pore in the n-th layer that the particle passed through being available.

The first subsection below presents a qualitative discussion of what the retention curve should look like; the subsections after that present computations for various layers models with specified selection rules.

2.1 The Plateau and the Drop-off, a General Description

The diagrams in this subsection illustrate why one would expect a plateau in the retention curve for $0 < k \ll K$ (the first few particles), followed by a significant drop-off after the filter has retained some critical number of particles. The assumptions for this subsection are

- 2 pore sizes, 1 (intermediate) particle size.
- $N = 10$ layers.
- $M = 100$ pores per layer.
- a random (equally probable) distribution of the two pore sizes.
- the spread is three pores (the one directly below and the ones on either side of it), and this spread is achieved using the *Left-Middle-Right (LMR) selection rule* (described next).

Under the LMR rule, the particle selects between the three closest pores below it. However if either the left or right pore is blocked, then the particle bypasses the blocked pore and continues in the given direction until it finds an unblocked pore. If the middle pore is blocked then the particle will chose to move either left or right. Thus, as long as the entire layer is not blocked, there will always be either 2 or 3 options for the next pore.

Figure 2 shows a representative 10-layer, 10-pore portion of a filter satisfying the assumptions above. Since roughly half of the pores are large, the filter appears to be fairly open. But Figure 3

```
### ####     ##     #### ####     ##     #### ###### ####-----#### ###
#     ##     #### ###### ####     #### ####-----#### ####-----##-----#
#-----##     ##     ##     #### ####-----##-----##-----##-----#### ###
### ###### ####     ##     #### ###### ###### ###### ####-----##-----#
###x###### ###### ####     #### ####xxxxx##xxxxx#### ###### ###### ###
#xxxxx####x###### ###### ####     ####x####xxxxx##xxxxx##xxxxx##xxxxx#
#xxxxx##xxxxx##xxxxx##     #### ####-----##xxxxx#### ####xxxxx####x###
#xxxxx##xxxxx##     ##     #### ####-----##-----##xxxxx##xxxxx####x###
###x###### ####     #### ####-----#### ###### ###### ####xxxxx##xxxxx#
#xxxxx##     #### ###### ###### ###### ####xxxxx##xxxxx####x######x###
```

Figure 3: The same portion of a cross section as in Figure 2 Again hash (or number) signs # represent the filter walls, and blank spaces, the pores themselves. In this diagram, the spread is three. Dashes ----- indicate large pores which lead only to small pores for the initial particle. In addition, pores filled with x are unreachable by the first particle, and unlikely to be reached by the first few particles.

shows that this is not the case, at least not for the first several particles entering the filter. In particular, pores filled with x are unreachable by the first particle into the filter, and are unlikely to be reached the first several particles. Pores filled by dashes ----- are reachable, but lead only to small pores when the three-pore spread rule is used. So the first particle to enter a dashed pore will be trapped, and the first several particles entering dashed pores are all likely to be trapped by the filter. This implies that the filter is much less open then it may have initial appear. In fact, the number of large pores in each layer which are initially part of a path through the filter (4, 3, 3, 2, 1, 1, 1, 2, 1, 1) is always less than half, and for half the layers there is only one. If the number of layers N was much greater than ten, there would have likely not been any through-paths at all for the first several particles (though in three-dimensional space, the filter would need many more layers to achieve this effect). All of this suggests a plateau in the retention curve for the first few particles entering the filter. And although this argument is heuristic, it could be made mathematically exact.

As particles beginning to fill a significant percentage of the small pores, a significant number of the blocked pores (either xxxxx or -----) will open up because of the spread rule that allows particles to bypass filled small pores. This means that later particles "see" a significantly larger number of large-pore paths that make it through the entire filter. As a result, the retention curve drops off dramatically.

2.2 Layer Computations

2.2.1 A First Layer Model

In this subsection, each pore in the filter is assigned a randomly determined width. A log normal distribution is used with a mean of 0.0 and a standard deviation of 0.5. This gives a mean pore width of 1.0. The maximum pore size allowed is chosen to be 3.0, and the probabilities are clipped at this value. For each test run, $K = 100,000$ particles with constant diameter of 1.5 flow through the filter.

Figure 4: The media: The red blocks represent a blocked pore, while the shade of grey represents the width of the pore: the darker a pore the wider it is.

In these computations, the spread is again three, and this spread is again achieved using the Left-Middle-Right selection rule (descibed above). The probability of selecting a given pore is now weighted by both the width of the pore and the lateral distance that needs to be travelled in order to get to that pore. The flow is taken to be poisseuille flow, meaning that it is proportional to w^4/l. where w is the width of the pore and l the lateral distance travelled. The middle pores are also weighted over the external pores.

The collection of images in Figure 4 shows how a piece of filter evolves over time. These images show the filter media itself for five different values of k (k = [WE NEED THE VALUES.]). The red blocks represent a blocked pore, while the shade of grey represents the width of the pore: the darker a pore the wider it is. The five images make clear how the narrower channels fill from the top down.

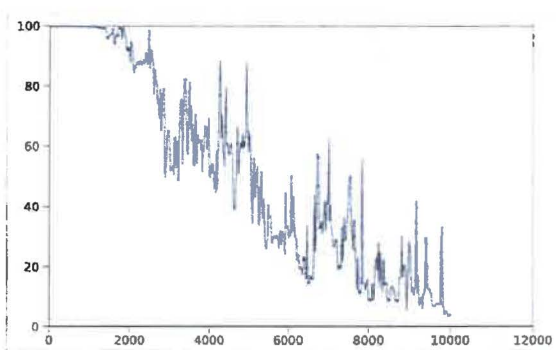

Figure 5: A noisy retention curve resulting from modelling too small a section of a filter. Here $M = 25$ pores per layer, and $N = 20$ layers.

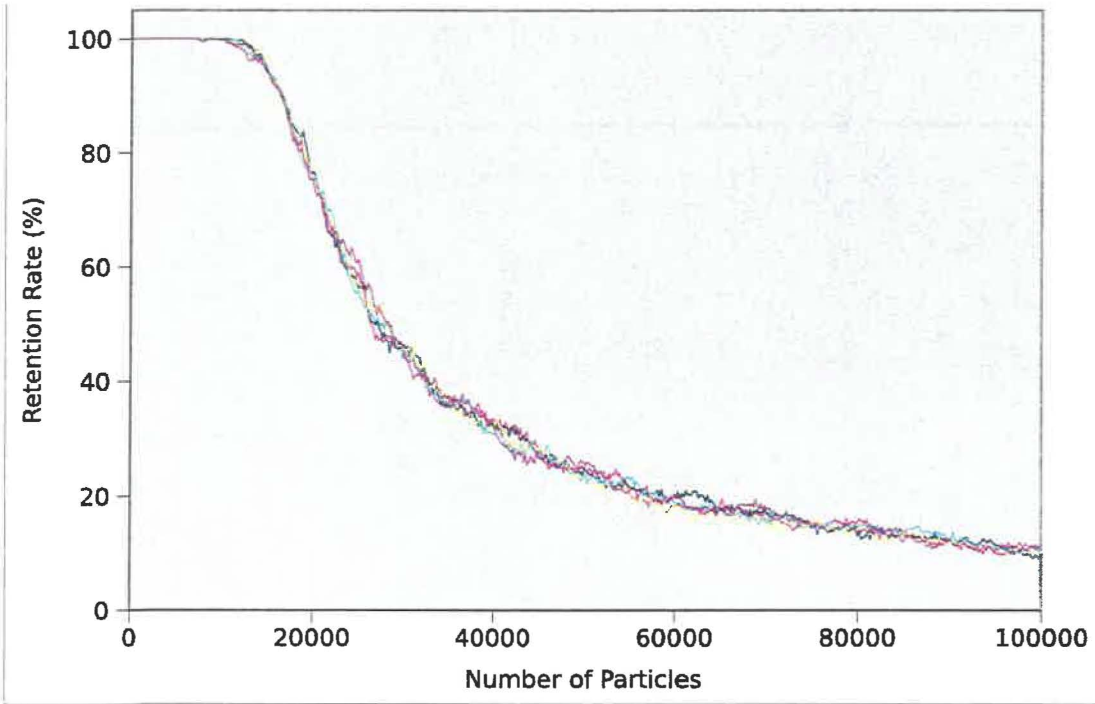

Figure 6: Five simulation runs on a filter with $M = 250$ and $N = 20$.

Noise: The next image (Figure 5) shows noise in the retention curve. This noise is due to the nature of the LMR rule. With the LMR rule, clogging a pore can increase the retention of the filter. By clogging one pore, another further out is opened up. This new pore may lead to a part of the filter that has a relatively high number of small pores. Thus there are now a number of newly available locations for particles to become trapped, and there is a jump in the retention rate of the filter, leading to noise (instability) in the graphs.

There is considerable noise when simulations are done on filter with a small numbers of pores: having only 500 pores results in a considerable amount of noise, while 5000 pores leads to much smoother retention curves. Figure 5 demonstrates this issue; here $M = 25$ pores per layer, and $N = 20$ layers, meaning that there are 500 total pores.

Simulation Consistency: In Figure 6, one porous filter was generated and then 5 separate simulation runs were conducted on this single filter. The porous filter has 5000 pores ($M = 250$ and $N = 20$). Again for each test, $K = 100,000$ and each particle has a constant diameter of 1.5. While there are some discrepancies, it is evident from the graph that the five tests are quite consistent. Again increasing the number of pores would decrease the noise and improve this consistency. Also using more test particles might further improve the measurement of the filter retention curve, and thereby improve the data.

A different consistency issue arises when constructing filters. Will two different filters generated with the same parameters have similar retention graphs? To explore this issue, three similar simulations were run, and the results are shown in Figure 7. As in the previous consistency test,

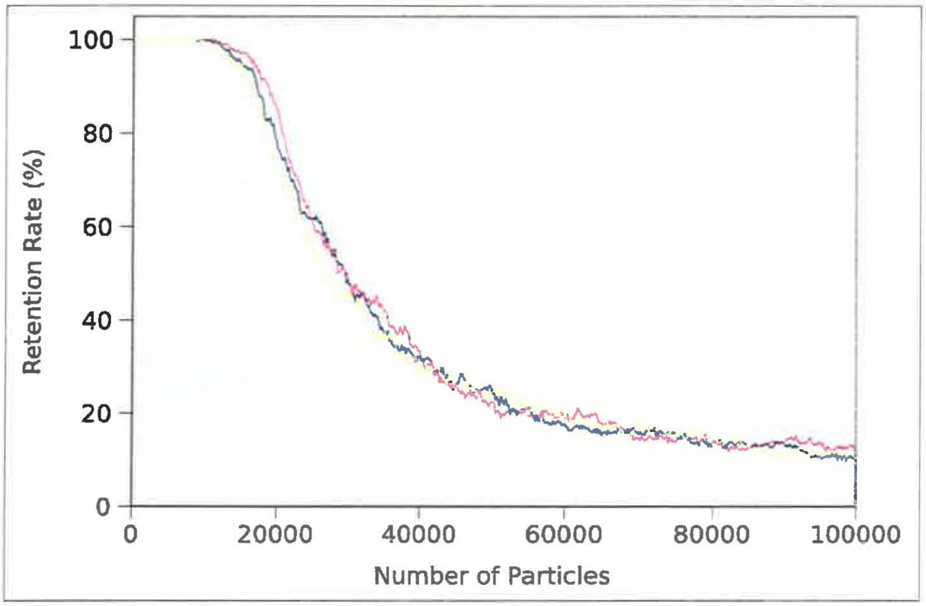

Figure 7: Three simulation runs on three separate filters which were generated using the same parameters.

here the graphs are relatively close, and again increasing the number of pores and/or particles should cause the differences to decrease.

Dependence on Particle Width and Width Distribution: For simulations in Figure 8, one porous filter was generated and tested three times. In each test, all particles flowing through the filter had a distinct, constant diameter. The porous filter again had 5000 pores ($M = 250$ and $N = 20$). For each test 100,000 particles were sent through the filter, and the retention rate was tested once every 200 particles. As expected the smallest diameter particle had the lowest retention rate. However the graphs for the 1.5 and 2.0 diameter are quite similar, having the same point at which their curves drop off from 100% retention. There is also increased noise in the graph for the largest diameter particles.

Finally, Figure 9 presents a pair of simulations with two distinct log normal particle volume distributions. In the first test the mean particle diameter was approximately 1.0, in the second, approximately 1.5. In these simulations the fluctuations discussed earlier have returned, particularly for the larger of the two particle diameters. Presumably, as was the case for a fixed particle diameter, if the number of pores and/or particles is increased, then these fluctuations would shrink.

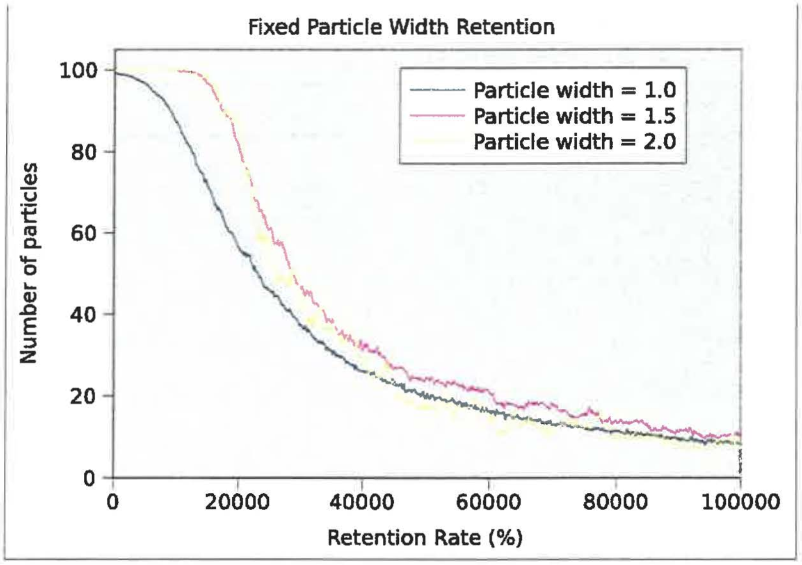

Figure 8: Computations for a single filter using three distinct particle diameters: 1.0, 1.5, 2.0.

2.2.2 A Second Layer Model

An alternate model for computing filter retention can be formulated by modifying the selection rules for particle movement between layers. This subsection details a different set of selection rules, in addition to modifications in the inclusion of the flow physics in computing the selection probabilities.

Selection Rules: As particles pass through a layer, they are restricted in choosing a given number of pores in the next layer of the filter through which to flow. As in the previous model, the spread in this model is restricted the the three nearest pores in the next layer (one to the left,

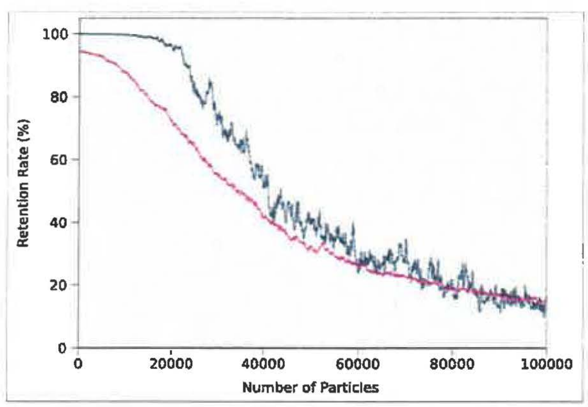

Figure 9: Computations for two distinct log normal particle volume distributions.

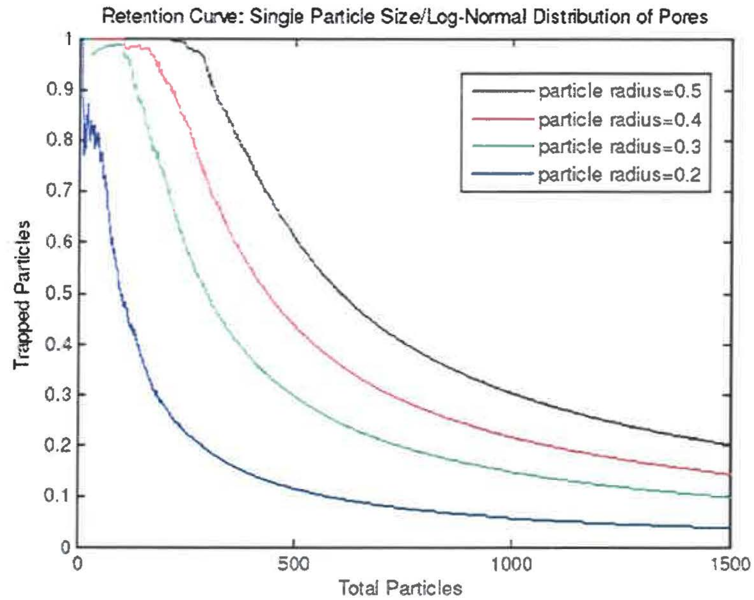

Figure 10: Equal probability selection retention curves for various entering particle sizes

one directly below, and one to the right), These three pores will be refered to as *daughter pores*. The particle has a probability of proceeding through any one of the three daughter pores, and this probability, presumably, should be based on the size of the pore and its distance from the source pore in the previous layer (different cases to be discussed further). Again this is the same as in the previous model.

The difference between this model and the previous one in regard to the selection rule is how blocked pores are handled. When one of the three pores gets clogged, then on the next pass a particle only has two pores to choose from. If all three pores become blocked, then the source pore is also shut down as particles would not be able to proceed through the filter. This process then continues until all of the small pores are blocked and the filter fails.

Equal Flow Probabilities: The initial and most primitive model treats pore selection with equal probability. Neither the pore size, nor the lateral distance of the pore from its source pore affects its selection. Effectively, once a particle passes through the source, it spreads with equal probability.

Figure 10 below shows a comparison of the retention curves when individual particles of a given size are passed through a filter having a log-normal distribution of pore sizes. The trend of the curves is to steepen as the particle size is reduced. This result is intuitively clear as smaller entering particles pass through a filter more easily, and hence the retention falls off more quickly.

Figure 11 shows a comparison of the retention curves when additional lateral nodes are inserted as possible daughter pores. The curves steepen slightly as nodes are added simply because there are more options for particles to escape. The effect in the equal probability case, however, is mostly negligible.

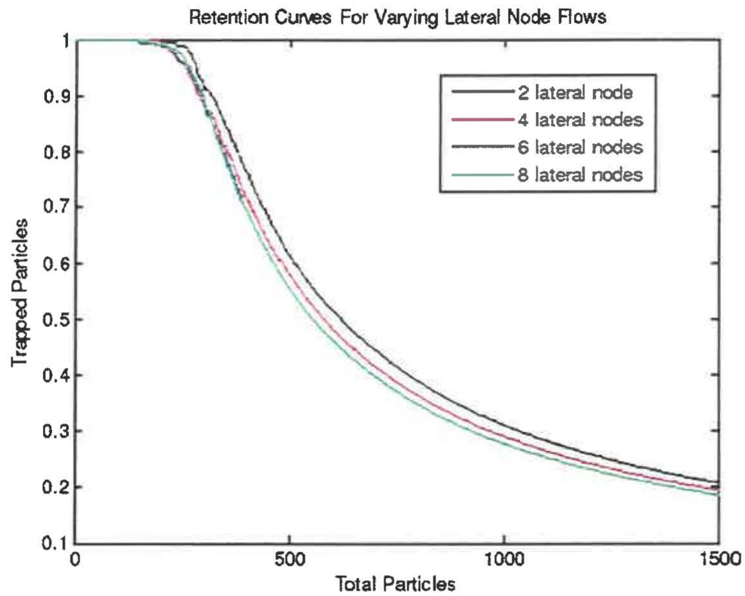

Figure 11: Retention curve trend as a function of added daughter pores.

Pore Size Based Flow: The refined model treats passage through a pore as channel flow. Hence, larger pores have more favorable passage because the volumetric flow rate through a channel goes as r^4 (where r is the radius of the channel). The probability of passing through each given daughter is found with the following formula,

$$P_i = \frac{r_i^4}{\sum_i r_i^4}. \tag{2}$$

This case, of course, makes it easier for particles to pass through the filter because larger pores are more favorable paths and fewer particles are trapped in large pores.

Figure 12 below is a comparison of the retention curves resulting from equal probability and pore size based probability selection rules. Again, the simulation uses a single particle size and a log-normal distribution of pore sizes. Notice that curve corresponding to pore size based retention is steeper than that of equal probability selection. This is the case because if the flow is modeled as channel flow, larger pores have more favorable selection, and particles escape the filter more easily.

Pore Size and Lateral Distance Based Probability: The effect of lateral distance (D_i) is added to the model by penalizing pores at great lateral distances from the source. The daughter pore immediately below the source would have no penalty and a daughter pore further away (large lateral distance) would have a larger penalty. This discourages particles from traveling great lateral

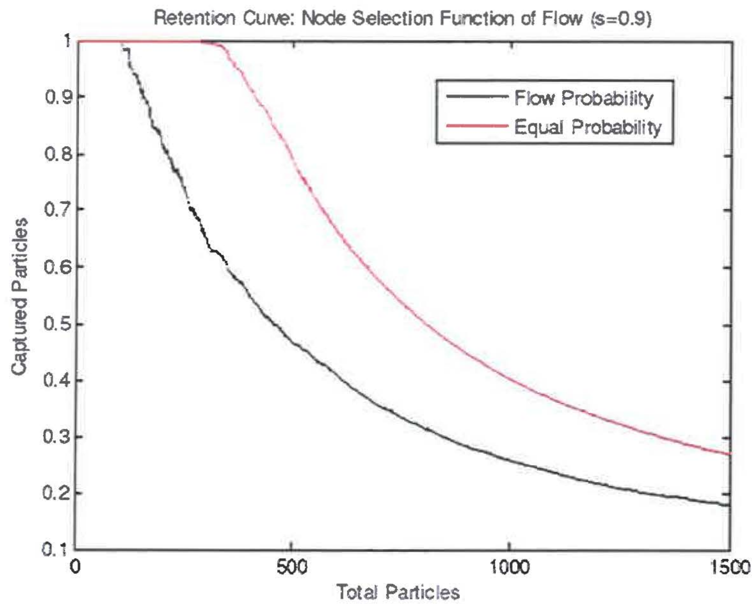

Figure 12: Comparison of retention curves resulting from equal probability and size based selection rules.

distances to reach pores. The new probability is then computed as follows,

$$P_i = \frac{r_i^4 D_i}{\sum_i r_i^4 D_i}$$
$$D_i = \frac{d_t - d_i}{d_t}, \tag{3}$$

where d_t is the maximum distance a particle can travel from the source node, and d_i is the actual lateral distance of the daughter pore from the source.

Notice that if $d_i = 0$ (referring to the pore just underneath the source), then $D_i = 1$ and there is no penalty. If $d_i = d_t$, then $D_i = 0$ and there is no chance of particles reaching the pore at distance d_t. Practically, d_t should be taken to be larger than the distance to the furthest daughter pore because if it is not, then the probability of reaching that daughter is always zero. In the model generated for gore, d_t is left as a parameter.

Figure 13 below shows a comparison of the retention curve resulting from all three physical cases. Notice that there is a minor influence to the rate of retention decay when a lateral distance penalty is added to the pore size based selection rules. The more interesting result is in Figure 14 which shows the retention curves converging to a single curve as additional daughter pores are allowed in selection. This happens because of the lateral distance penalty. Ultimately, pores very far away from the source have little chance of acceptance, so adding additional daughters at large distances from the source adds little effect.

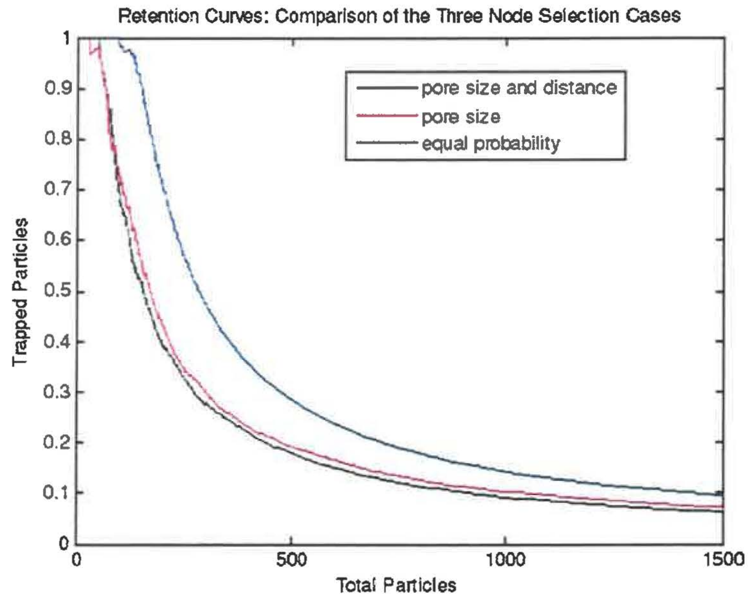

Figure 13: Retention curve comparison of all three physical cases.

Differences Between the First and Second Models:

- The previous model throws many particles at a filter at a certain level of clogging, checks the average retention, then clogs a pore and repeats the process. This model simply throws pores at the filter and computes the retention in real time.
- The previous model allows for a particle to bypass blocked pores; this model allows for a finite spread (the number of daughter pores in the spread being left as a parameter) but does not allow blocked pores to be bypassed.
- When putting in lateral distance penalties, the previous model measures this distance by counting bypassed pores. The current model measures this distance in terms of the mean pore size. Hence the functions used to compute probabilities when including lateral distances are different.

2.2.3 A Probabilistic Layer Model

Now let us consider three cases where the probability of moving through a given layer it proportional to the fraction of unblocked pores which are large. As in the previous section, first suppose that there is one particle size and two pore sizes. Also suppose the ratio of large pores to total pores is p_0. Note that this value is constant throughout the filtering.

For a specific particle, suppose it has passed the $(n-1)$-st layer, and let us consider its probability of passing the n-th layer. Let p_n denote the portion of large pores in the n-th layer. If we look at one pore, its probability of being a large one is p_n. In this case, let us use the following spread

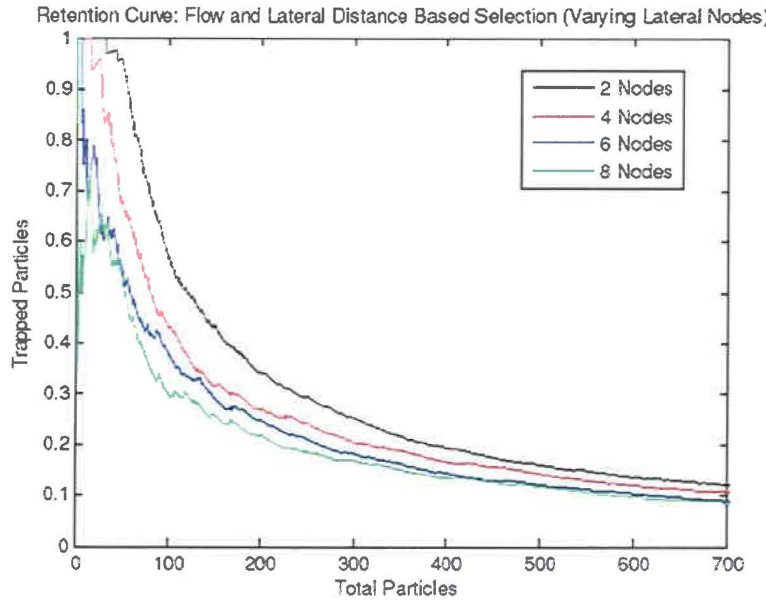

Figure 14: Effect of additional daughter pores on retention curves when selection incorporates both pore size and lateral distance from source.

rule: suppose the particle has probability 1/2 of going straight down and probability 1/4 of going either left and right respectively. Then the probability of the particle passing the n-th layer is $\frac{1}{2}p_n + \frac{1}{4}p_n + \frac{1}{4}p_n = p_n$. So the probability that the particle passes through the n-th layer does not depend on the spread rule in this case.

Therefore we suppose there are N layers, and the probability for a particle to pass each layer is given by $p_1, p_2, \ldots, p_N$, where again p_n is the portion of large pores in the n-th layer. The probability that the particle passes the filter is $p_1 p_2 \cdots p_n$, and the probability of getting stuck in the n-th layer is $p_1 \cdots p_{n-1}(1 - p_n)$.

After each particle passes through the filter, one must update the values of p_n. We replace p_n by

$$\begin{aligned} p_n \;\leftarrow\; & p_n \cdot \Pr(\text{last particle was not stuck in the } n\text{-th layer}) \\ & + p_n' \cdot \Pr(\text{last particle was stuck in the } n\text{-th layer}) \end{aligned}$$

where p_n' (the new portion of large pores in the n-th layer if last particle was stuck there) is given by

$$p_n' = \frac{M \cdot p_0}{M \cdot p_0/p_n - 1}$$

In (2.2.3), M is the initial total number of pores in each layer, $M \cdot p_0$ is the number of large pores in each layer (a number that does not change), and $M \cdot p_0/p_n$ is the number of available pores—pores that are not blocked by any particle. When a particle blocks a small pore, the number of available

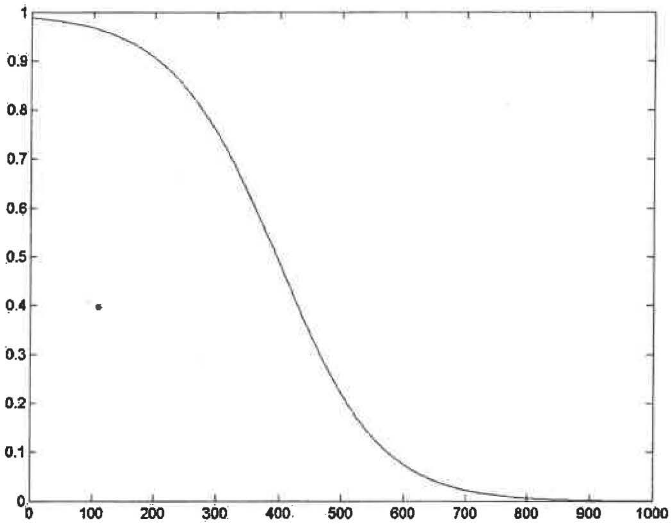

Figure 15: A retention curve for a simple probabilistic computation.

small pores is reduced by one and becomes $M \cdot p_0/p_n - 1$. Finally the two probabilities in (2.2.3) are

$$\begin{aligned} \Pr(\text{last particle was stuck in the } n\text{-th layer}) &= p_1 \cdots p_{n-1}(1-p_n), \quad \text{and} \\ \Pr(\text{last particle was not stuck in the } n\text{-th layer}) &= 1-[p_1 \cdots p_{n-1}(1-p_n)]. \end{aligned} \tag{4}$$

For the computations in this subsection, there are $N = 20$ layers, $M = 100$ pores per layer, and $K = 1000$ particles. Initially 80% of the pores are large pores, so $p_0 = 0.8$. A retention curve obtained using these values is shown in Figure 15.

Next we examine a more complicated case where pore size is assumed to satisfy a lognormal distribution and there are two particle sizes (with half the particles being of each size).

Let a_1 and a_2 denote respectively the small and large particles sizes. This separates the pores

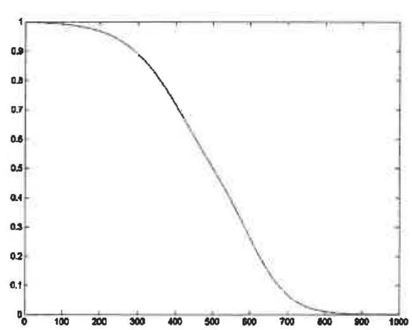

Figure 16: A retention curve for a second probabilistic computation. Note that the x-axis is not the number of particles K, but rather $K/2$.

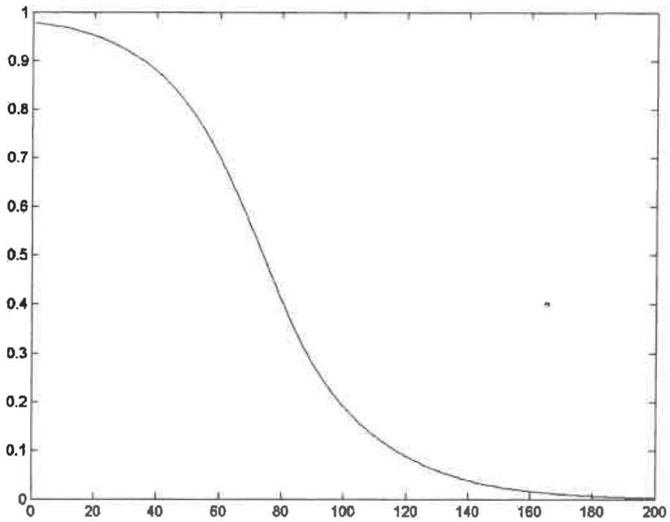

Figure 17: A retention curve for a third probabilistic computation. Here the x-axis is not the number of particles K, but rather K/N.

into 3 different classes: large ones that both large and small particles can go though, medium-sized ones that small particles can go though but large ones can not, and small ones that no particles can go though. Since the distribution of pore size is given, the portion of each of the 3 classes can be calculated.

Since half of the particles are large and half small, it is reasonable to simplify the computations by alternating the large and small particles. After each particle, the algorithm updates the portions of pores of each size in each layer. As in the previous case, there are $N = 20$ layers and $M = 100$ pores per layer, but now we use $K = 2000$ particles. The size of the small particles is 0.5; the size of the large particles is 1.0. The distribution of pore sizes is Lognormal(0,1). A computational run with these values yielded the retention curve in Figure 16.

Finally consider a general case where both pore size and particle size satisfy lognormal distributions. Discretize the particle size distribution into I intervals, and assume that the particle size has the same probability $1/I$ of being in each interval. Pick one size in each interval as the representative. Thus there are I different particle sizes, and they separate pores into $I + 1$ classes. Assume that representative particles enter the filter in turn, so that one of each of the I sizes enters the filter before another of a given size enters. In this case there are $N = 10$ layers, $M = 100$ pores per layer, $K = 2000$ particles, and $I = 10$ intervals. The pore size distribution is Lognormal(0,2), and the particle size distribution is Lognormal(0,1). A retention curve for this case is given in Figure 17.

3 Continuum Modelling

3.1 The Simplest Approach

This section presents a simple continuum model for the case where there are two pore sizes and one intermediate particle size. Let $p^{(k)}$ be the probability that the k-th particle is trapped in the filter. Then

$$p^{(k+1)} = p^{(k)}(1 - p^{(k)}) + \frac{(p^{(k)} - \delta)}{1 - \delta} p^{(k)} \tag{5}$$

where δ is the probability of getting trapped in any particular pore. Since M is the number of pores per layer, then $\delta \sim 1/M$ and δ is assumed to be uniform throughout the filter. In words, this equation says that the probability that the $k+1$-st particle is trapped in the filter is the same as the probability that the k-th particle is trapped given that the k-th particle made it through, plus a reduced probability of being trapped given that the k-th particle was trapped. Let $s := k\delta$; this is in some sense a scaled measure of time and should be thought of as a continuous parameter. and linearize the $1 - \delta$ factor in the denominator. Then

$$p(s+\delta) = p(s)(1 - p(s)) + p(s)(p(s) - \delta)(1 + \delta) + O(\delta) \tag{6}$$

which implies

$$\frac{p(s+\delta) - p(s)}{\delta} = p^2(s) - p(s) + O(\delta). \tag{7}$$

Taking the limit as $\delta \to 0$, one obtains the following ODE for p:

$$\frac{dp}{ds} = p^2 - p. \tag{8}$$

The solution of (8) is easy to obtain by separation of variables:

$$p(s) = p(k\delta) = \frac{1}{1 + \epsilon e^{k\delta}}. \tag{9}$$

where ϵ is a constant of integration. Assuming that initially the filter is trapping the vast majority of the particles, one has that $0 < \epsilon \ll 1$.

Now suppose, similar to supposition in subsection 2.2.2, that the probability of making it through a pore of radius r is

$$\frac{r^4}{\alpha} f(r) \tag{10}$$

where $f(r)$ is the normalized distribution of pore sizes and $\alpha := \int_0^\infty r^4 f(r)\, dr$. Then the probability that the first particle with radius R makes it through a single layer is

$$\int_R^\infty \frac{r^4}{\alpha} f(r)\, dr \tag{11}$$

and thus the probability of a particle with radius R making it through n layers is

$$\rho = \left(\int_R^\infty \frac{r^4}{\alpha} f(r)\, dr \right)^n \tag{12}$$

So this allows one to write an expression for the integration constant ϵ based on this initial probability:

$$\epsilon = \frac{\rho}{1 - \rho} \tag{13}$$

A representative plot of the probability distribution $p(s)$ is shown in Figure 18:

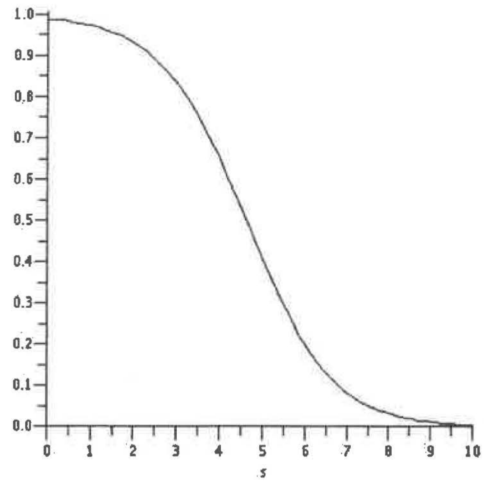

Figure 18: A representative plot of the probability distribution $p(s)$ with $\epsilon = 0.01$.

3.2 A Second Approach

The previous subsection makes the assumption that the probability of a particle getting trapped in any particular open pore does not change as pores become blocked. In fact, as more pores become blocked, the probability of a particle getting trapped in a particular pore should increase. Now we can define δ^k as the probability of a particle getting trapped after k particles have already been introduced into the system. One can also define ω_s^k as the number of small paths open after k particles have been deposited into the system and ω_b as the number of larger paths open. Then

$$\delta^k = \frac{1}{\omega_s^k + \omega_b} \tag{14}$$

which we can rewrite as

$$\delta^k = \frac{1}{\omega_b} \frac{1}{1 + \frac{\omega_s^k}{\omega_b}} \tag{15}$$

Using a similar argument we can conclude that the probability of the $(k+1)^{st}$ particle becoming trapped is

$$p^{k+1} = (1 - p^k)p^k + p^k \frac{p^k - \delta^k}{1 - \delta^k} \tag{16}$$

Then using linearization, one finds

$$p^{k+1} = (1 - p^k)p^k + p^k(p^k - \delta^k)(1 + \delta^k) + O(\delta^k) \tag{17}$$

which implies, as before,

$$\frac{p^{k+1} - p^k}{\delta^k} = (p^k)^2 - p^k + O(\delta^k) \tag{18}$$

Using equation (12), one can obtain the following approximate differential equation:

$$\frac{dp}{ds} = \frac{p^2 - p}{1 + \phi} \tag{19}$$

where $s = \frac{k}{n}$ and $\phi := \frac{\omega_s^k}{\omega_b}$. Using the substitution $p^k = \omega_s^k \delta^k = \frac{\phi}{1+\phi}$, we obtain

$$\frac{d\phi}{ds} = -\frac{\phi}{1 + \phi} \tag{20}$$

The solution to this ODE is known as the Lambert W function, defined implicitly by

$$\phi e^{\phi} = Ae^{-s}, \tag{21}$$

where A is a constant of integration which can be determined from the initial probability of a particle getting trapped, $1 - \rho$, given by (12). We find that

$$A = \frac{1-\rho}{\rho} \exp\left(\frac{1-\rho}{\rho}\right). \tag{22}$$

3.3 Two particle sizes

We now extend the problem to consider two particle sizes: small particles and large particles. With two particle sizes the available pores are partitioned into three categories:

- *Small pores*: both small and large particles will become trapped.
- *Medium pores*: large particles are trapped, but small ones pass through.
- *Big pores*: both small and large particles escape.

We shall make the simplifying assumption that large particles never become trapped in small pores. As the particles enter the filter a proportion, b of them will be big. Define

$$\begin{aligned} p^k &= P(k^{th} \text{ particle is retained} \mid k^{th} \text{ particle is big}) \\ q^k &= P(k^{th} \text{ particle is retained} \mid k^{th} \text{ particle is small}). \end{aligned}$$

Next define the probability of a large particle following a particular path as δ, and as in section 3.1, assume that δ as constant. We also assume that the probability of a small particle following a particular path is constant and define this by ϵ_s. When a large particle blocks a medium-sized pore it will reduce the total number of escape paths available for a small particle. We shall model this by assuming that the fraction of escape paths for the small particles is reduced by a fraction $(1 - \epsilon_b)$, where ϵ_b is constant Note that, since the total number of paths is large, δ, ϵ_s and ϵ_b are all small. For the large particles we use the same conditioning argument as in section 3.1; however, we must now also condition on whether the previous particle was big or small. One finds that

$$p^{k+1} = b\left((1 - p^k)p^k + p^k \frac{p^k - \delta}{1 - \delta}\right) + (1 - b)p^k, \tag{23}$$

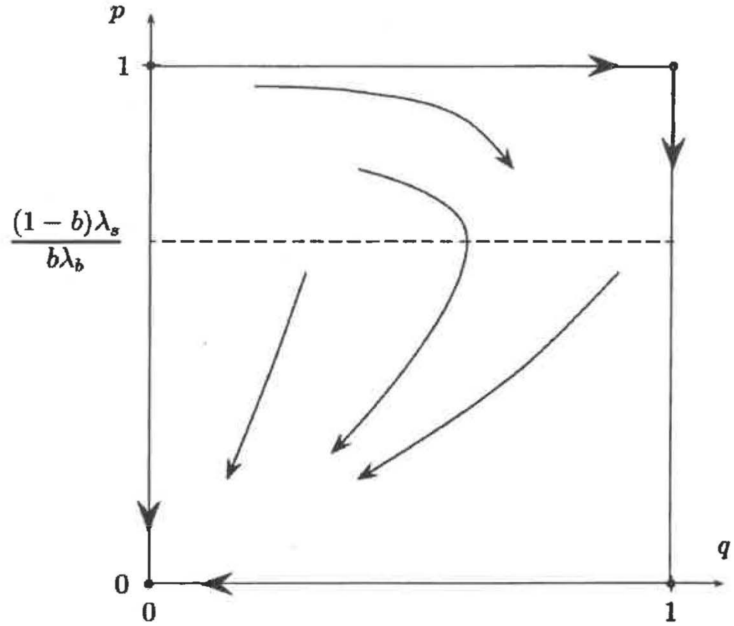

Figure 19: The phase-plane for the equations (34), (35). The dots represent steady states and the dashed line along with $p = 0, 1$ and $q = 0, 1$ are nullclines.

and since δ is small, we may apply the same argument as in section 3.1 and find that

$$\frac{dp}{ds} = b(p^2 - p)\,. \tag{24}$$

If we define the number of retaining paths for the k^{th} particle, given that the k^{th} particle is small, by S^k, and the number of trapping paths for this particle to be B^k then

$$q^k = \frac{S^k}{S^k + B^k}. \tag{25}$$

If the k^{th} particle is big and gets trapped then

$$B^{k+1} = (1 - \epsilon_b)B^k. \tag{26}$$

By applying our conditioning argument on the k^{th} particle we find

$$q^k = b\left((1-p^k)q^k + p^k\frac{S^k}{S^k + (1-\epsilon_b)B^k}\right) \tag{27}$$

$$+(1-b)\left((1-q^k)q^k + q^k\frac{q^k - \epsilon_s}{1-\epsilon_s}\right). \tag{28}$$

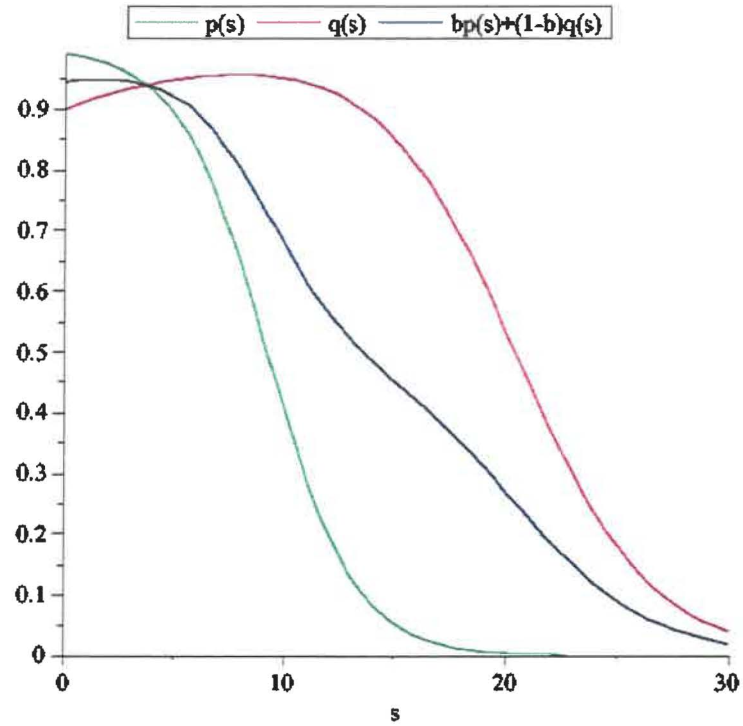

Figure 20: Retention curves for the two particle-size problem. Parameters are $b = 1/2$, $\lambda_b = 1$, $\lambda_s = 2/3$ and initial conditions are $p(0) = 0.99$, $q(0) = 0.9$.

We note that

$$\frac{S^k}{S^k + (1-\epsilon_b)B^k} = \frac{S^k}{S^k\left(1 + \frac{(1-\epsilon_b)(1-q^n)}{q^n}\right)} \tag{29}$$

$$= \frac{q^n}{1-\epsilon_b(1-q^n)}. \tag{30}$$

Since ϵ_s and ϵ_b are both small we linearize to find

$$q^k = b\left((1-p^k)q^k + q^k p^k\left(1+\epsilon_b(1-q^k)\right)\right) \tag{31}$$

$$+(1-b)\left((1-q^k)q^k + q^k(q^k-\epsilon_s)(1+\epsilon_s)\right). \tag{32}$$

Now introduce the parameters

$$\lambda_s = \frac{\epsilon_s}{\delta}, \quad \lambda_b = \frac{\epsilon_b}{\delta},$$

both assumed to be neither small nor large, i.e. ϵ_s, $\epsilon_b = O(\delta)$. These parameters help to describe the structure of the porous media. By again introducing $s = k\delta$ and applying the argument of section 3.1 we find

$$\frac{dq}{ds} = b\lambda_b pq(1-q) + (1-b)\lambda_s(q^2-q). \tag{33}$$

We are left with the pair of equations:

$$\frac{dp}{ds} = b(p^2 - p), \quad (34)$$

$$\frac{dq}{ds} = b\lambda_b pq(1-q) + (1-b)\lambda_s(q^2 - q). \quad (35)$$

We can gain some insight into the behaviour of (34), (35) by looking at the phase plane. There are steady states when $p = 0, 1$ and $q = 0, 1$, with the only possible stable steady state at $p = 0, q = 0$ i.e. when no particles are retained. When

$$\frac{(1-b)\lambda_s}{b\lambda_b} < 1, \quad (36)$$

it is possible for the retention rate of small particles to increase, provided the retention rate for large particles is large enough, i.e. the large particles can screen the small particles and increase the effectiveness of the filter. Since the retention rate for large particles must always decrease this effect is only temporary and eventually the retention rate for the small particles must drop.

4 Network modeling

In this section, we explore the mathematics underlying a network model for simple sieving. The main disadvantage to this model is that one disregards all hydrodynamic effects in the porous material. The advantage is that one can distill some essential, predictive mathematics from the problem without resorting to experimentation of specific parameters. The material properties are characterized by the distribution of possible paths through the porous material.

We begin by representing the porous material as a connected, directed graph with edges being passages through which fluid can flow and vertices corresponding to junctions where three or more passages meet. The high pressure side of the porous substance can be considered to be a single vertex which will be referred to as the *source* and similarly the low pressure side can be considered a single vertex called the *sink*. A schematic diagram of a simple porous medium is shown in Figure 21.

Fluid will flow along graph edges from the high pressure source to the low pressure sink. The fluid carries with it small particles which may or may not be large enough to pass through any given passage. Therefore, particles reaching an edge corresponding to a passage that is narrower than the particle size can be considered a *clog*. The particle will go no further, and the edge is no longer available to transport fluid. An *unobstructed path* through filter is defined to be a single route through the porous material from source to sink which does not reach a clog. An *obstructable root structure* is the collection of all paths leading from the source to an individual clog. An example of an unobstructed path and an obstructable root structure are shown in Figure 22.

If we know the probabilities of a particle passing through either an unobstructable path or an obstructable root structure, then we can develop a model for simple sieving. In developing this model, we make the following assumptions.

- A particle will enter an unobstructable path or an obstructable root structure with equal likelihood.
- If a particle passes into an obstructrable root structure, fluid can no longer follow the paths comprising this structure but the hydrodynamic properties of the medium are otherwise unaltered.

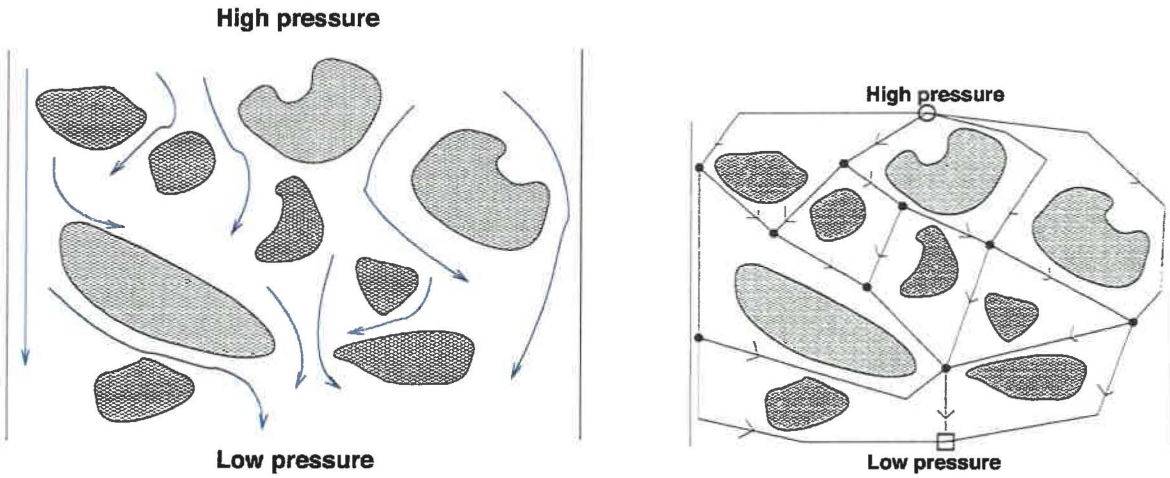

Figure 21: Decomposition of a simple porous structure (left) into a directed graph (right). The source is indicated by a circle, and the sink by a square.

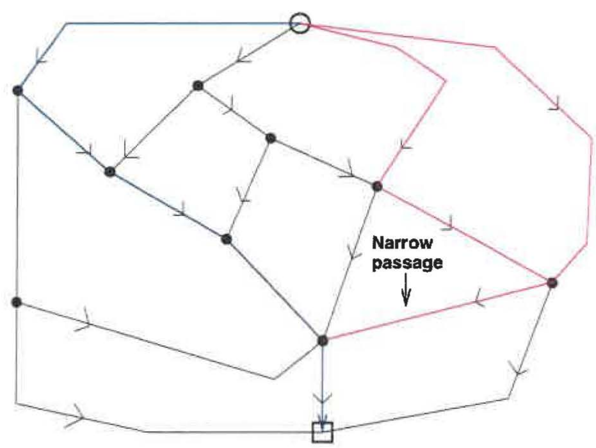

Figure 22: Description of different categories of paths. An unobstructed path is shown in blue; an obstructable root structure, in red.

Our approach is similar that of Lee and Koplik [4] except that they perform their simulations and analyses on a regular array while we perform ours on an arbitrary directed graph. However, we require stronger assumptions, particularly the equal likelihood of all possible unobstructable paths and obstructable root structures.

With these assumptions, the probability of a particle being trapped in the medium is

$$p = \frac{o}{o+u} \tag{37}$$

where o is the number of obstructable root structures and u is the number of unobstructable paths. Notice that the form of this equation is very similar to (14) in our continuum analysis above. Also notice that o changes with time, but u does not. Thus, the network probability p changes when a particle is trapped and one obstructable root structure is eliminated, but if a particle is not trapped (with probability $1-p$), the probability does not change.

If we suppose that particles approach the medium one at a time and move into a path at random, we can refer to o_k as the expected value of o after k particles have moved through the system.

$$o_{k+1} = p_k(o_k - 1) + (1 - p_k)o_k \tag{38a}$$

$$= -p_k + o_k \tag{38b}$$

$$p_k = \frac{o_k}{o_k + u} \tag{38c}$$

If we define

$$\phi_k = \frac{o_k}{u} \tag{39}$$

then we can see that

$$p_k = \frac{\phi_k}{1+\phi_k}. \tag{40}$$

Substituting (39) and (40) into (38),

$$\phi_{k+1} = -\frac{\phi_k}{u(1+\phi_k)} + \phi_k. \tag{41}$$

Hence,

$$\frac{\phi_{k+1} - \phi_k}{1/u} = -\frac{\phi_k}{1+\phi_k}. \tag{42}$$

We can let $s = k/u$ and assume that u is large so that s can be approximated as a continuous variable describing the passage of time so that the discrete system can be approximated by a solution to the ordinary differential equation,

$$\frac{d\phi}{ds} = -\frac{\phi}{1+\phi}. \tag{43}$$

This is of course identical to Equation (20) in our continuum modelling, and again it has solutions of the form

$$\phi(s) = \exp\{-\mathrm{W}[\exp(-s-C)] - s - C\}, \tag{44}$$

where here W is again the Lambert W function. Therefore,

$$p = \frac{\mathrm{W}[\exp(-s-C)]}{1+\mathrm{W}[\exp(-s-C)]}. \tag{45}$$

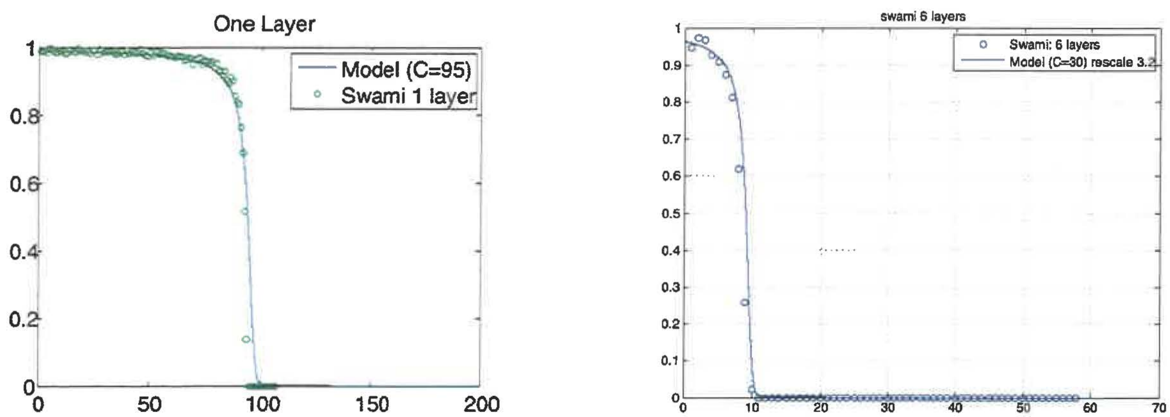

Figure 23: Comparisons between layer simulations and the network theory prediction for 1 layer (left) and 6 layers (right).

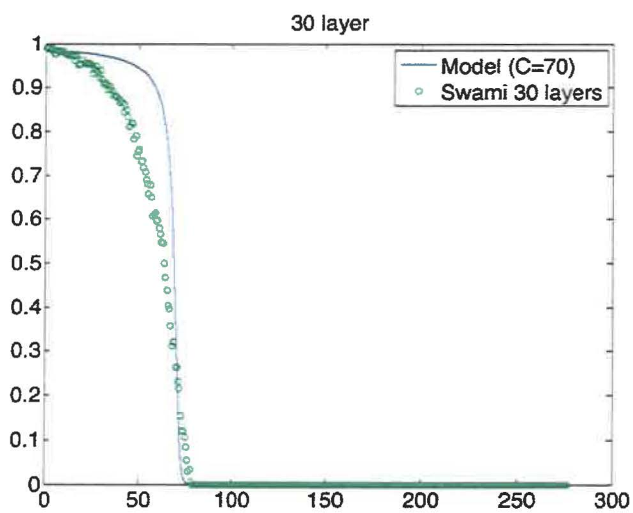

Figure 24: With 30 layers, the network theory fails because the equal probability assumption no longer corresponds to reality.

describes the retention curve as a function of time.

One of the great strengths of this model is that the complex filtration dynamics are reduced to an analytic expression with one free parameter C which characterizes the filter. One could argue that the characteristic timescale in (45) is another, but this should be determined by the particle density and the flow rate. We expect excellent agreement between theory and simulation of the layered model (*cf.* Section 2) when there is a single layer, but we expect the correspondence to erode as the number of layers increases because the equal likelihood assumption fails. In Figure 23, we fit C manually and find excellent agreement with simulations. With 30 layers, we see that we no longer capture the retention curve (Figure 24).

References

[1] Y.-I. Chang and H.-C. Chan, *Network simulation for deep bed filtration of brownian particales–a supplement*, Chemical Engineering Science **60** (2005), 2827–2831.

[2] S. Datta and S. Redner, *Gradient clogging in depth filtration*, Physical Review E **58** (1998), 1203–1206.

[3] W. Hwang and S. Redner, *Infiltration through porous media*, Physical Review E **63** (2001), 1–13.

[4] J. Lee and J. Koplik, *Simple model for deep bed filtration*, Physical Review E **54** (1996), 4011–4020.

[5] S. Redner and S. Datta, *Clogging time of a filter*, Physical Review Letters **84** (2000), 6018–6021.

[6] S.D. Rege and H.S. Fogler, *A network model for deep bed filtration of solid particles and emulsion drops*, AIChE Journal **34** (1988), 1761–1772.

[7] N. Roussel, T. Nguyen, and P. Coussot, *General probabilistic*, Physical Review Letters **98** (2007), 1–4.

[8] C. Shin, *Numerical simulation for particle penetration depth distribution in deep bed filtration*, Chemical Engineering Technology **29** (2006), 905–909.