Abstract

Membrane filters are widely-used in micro-filtration applications. The type of membrane used can vary widely depending on the particular application, but broadly speaking the requirements are to achieve fine control of separation, with low power consumption. The answer to this problem would seem obvious: select the membrane with the largest pore size and void fraction consistent with the separation requirements. However, membrane fouling (an inevitable consequence of successful filtration) is a complicated process, which depends on many parameters other than membrane pore size and void fraction; and which itself greatly affects the filtration process and membrane functionality. The challenge posed to the workshop was to devise mathematical models that can (i) account for the membrane internal morphology (internal structure, pore size & shape, etc.); and (ii) describe the fouling and separation.

1 Introduction

The Workshop explored several different modeling avenues, two of which are detailed in the following sections: (i) Darcy-type modeling, with the macroscopic membrane permeability based on the microscopic membrane pore characteristics; (ii) a local problem of particle capture within the membrane for different types of local geometry; (iii) Computational Fluid Dynamics (CFD) simulations of particle transport (coupled to various capture models) within membranes of simple internal structure; and (iv) general considerations of membranes with fractal internal structure.

The type of modeling most appropriate for a given situation depends on the type of membrane under consideration. Figure 1 shows several examples: (a) and (b) here might be better modeled as a system of channels or pores running through the membrane, while (c) and (d) are more like a series of nodes with thin, connecting fibrils—a so-called node-fibril microstructure. The pore-based Darcy models considered in §2 are most appropriate for membranes with microstructure of the kind seen in Fig. 1 (a), (b), while the computational fluid dynamics approach described in §3 (which considers flow with advection of microparticles around one or more obstacles, which model fibrils or nodes) is more appropriate for membranes with microstructure of the kind seen in Fig. 1 (c), (d).
The modeling of this section attempts to link the microscopic pore characteristics to the macroscopic permeability of a membrane filter, and to describe the flow through and fouling of a membrane filter. Throughout this section we assume that the membrane is flat and lies in the \((Y, Z)\)-plane, with unidirectional Darcy flow through the membrane in the positive \(X\)-direction. The membrane properties and flow are assumed homogeneous in the \((Y, Z)\)-plane, but membrane structure may vary internally in the \(X\)-direction (depth-dependent permeability) thus we seek a solution in which properties vary in \(X\) and in time \(T\). Throughout this section we use uppercase fonts to denote dimensional quantities; lowercase font will be dimensionless.

The superficial Darcy velocity \(U = (U(X, T), 0, 0)\) within the membrane is given in terms of the pressure \(P\) by

\[
U = -\frac{K(X, T)}{\mu} \frac{\partial P}{\partial X}, \quad \frac{\partial}{\partial X} \left( K(X, T) \frac{\partial P}{\partial X} \right) = 0, \quad 0 \leq X \leq D, \tag{1}
\]

where \(K(X, T)\) is the membrane permeability at depth \(X\). We consider two driving mechanisms: (i) constant pressure drop across the membrane specified; and (ii) constant flux through the membrane specified. In the former case the flux will decrease in time as the membrane becomes fouled; in the latter, the pressure drop required to sustain the constant flux will rise as fouling occurs. We will focus primarily on case (i) in this report, and so assume this in the following; our simulations for the constant flux scenario shown later require minor modifications to the theory, outlined in §§2.1.2, 2.2.2. With constant pressure drop, the conditions applied are

\[
P(0, T) = P_0, \quad P(D, T) = 0. \tag{2}
\]

The key modeling challenge is how to link the macroscopic membrane permeability \(K(X, T)\) to measurable membrane characteristics in order to obtain a predictive model. In this section we consider a simple model in which the membrane consists of a series of identical channels of variable radius \(A(X, T)\), which traverse the entire membrane. The basic setup is schematized in Figure 2: we consider a filtrate, carrying some concentration \(C\) of particles, which are deposited within the pore. We suppose the pores to be arranged in a square repeating lattice, with period \(2B\).

Mass conservation shows that the pore velocity, \(U_p\) (the cross-sectionally averaged axial velocity
within each pore), satisfies

$$(U_pA^2)_X = 0,$$  \hspace{1cm} \text{(3)}

while Darcy’s law for the superficial velocity $U$ within the pore gives

$$U = -\frac{\pi A^4}{8\mu(2B)^2} \frac{\partial P}{\partial X} = -\frac{\phi K_p}{\mu} \frac{\partial P}{\partial X} = -\frac{K}{\mu} \frac{\partial P}{\partial X},$$  \hspace{1cm} \text{(4)}

where $P$ is the pressure associated with the Darcy flow, $K_p = A^2/8$ is the permeability of the isolated pore and $\phi = \pi A^2/(2B)^2$ is the void fraction of the membrane. The pore and superficial velocities are related by

$$4UB^2 = \pi A^2 U_p$$  \hspace{1cm} \text{(5)}

by a simple flux-balance argument, consistent with (3). The model is completed by making assumptions about how particles are deposited within pores, with consequences for the particle concentration within the flow and for the pore radius. We propose a simple advection model

$$U_p \frac{\partial C}{\partial X} = -\Lambda AC,$$  \hspace{1cm} \text{(6)}

to be solved subject to specified particle concentration at the inlet,

$$C(0, T) = C_0.$$  \hspace{1cm} \text{(7)}

This model assumes that particles are deposited on the wall at a rate proportional to both the local particle concentration, and to the available wall circumference. The (dimensional) constant $\Lambda$ captures the physics of the attraction between particles and wall that is causing the deposition. The pore radius shrinks in response to the deposition: consistent with our deposition model we propose

$$\frac{\partial A}{\partial T} = -\Lambda \alpha C$$  \hspace{1cm} \text{(8)}

for some constant $\alpha$, which simply assumes that the pore cross-sectional area shrinks at a rate given by the total area of particles deposited locally (which was assumed proportional to $AC$ in (6)). The initial pore radius is specified throughout the membrane,

$$A(X, 0) = A_0(X).$$  \hspace{1cm} \text{(9)}
2.1 Scaling & nondimensionalization

Before presenting solutions we first nondimensionalize the model equations, to reduce the number of unknown parameters. We focus primarily on the case of flow driven by a constant pressure drop, §2.1.1 below, but briefly outline the difference in scalings when instead the flux is specified, in §2.1.2.

2.1.1 Specified pressure drop case

We nondimensionalize the model (2)–(9), using the scalings

\[ P = P_0 p, \quad X = D x, \quad C = C_0 c, \quad (A, B) = B(a, 1), \quad (U, U_p) = \frac{\pi B^2 P_0}{32\mu D} (u, u_p), \quad T = \frac{B}{\Lambda a C_0} t, \]

(10)
giving the following one-parameter dimensionless model for \( u(x, t), \ u_p(x, t), \ p(x, t), \ a(x, t), \ c(x, t) \):

\[ 4u = \pi a^2 u_p, \]

(11)
\[ u = -a^4 \frac{\partial p}{\partial x}, \quad \frac{\partial u}{\partial x} = 0, \]

(12)
\[ u_p \frac{\partial c}{\partial x} = -\lambda ac, \quad \lambda = \frac{32\Lambda \mu D^2}{\pi P_0 B}, \]

(13)
\[ \frac{\partial a}{\partial t} = -c, \]

(14)
with boundary and initial conditions

\[ p(0, t) = 1, \quad p(1, t) = 0, \quad a(x, 0) = a_0(x), \quad c(0, t) = 1, \]

(15)
where \( a_0(x) < 1 \) is a specified function.

Significant analytical progress may be made with this model. Equations (12) give the pressure \( p \) as

\[ p = u \int_x^1 \frac{dx'}{a^4}, \]

(16)
and then imposition of the condition \( p(0, t) = 1 \) gives the superficial Darcy velocity \( u(x, t) \) in terms of the pore radius \( a(x, t) \) as

\[ u = \left( \int_0^1 \frac{dx}{a^4} \right)^{-1}, \quad \text{hence} \quad u_p = 4 \left( \pi a^2 \int_0^1 \frac{dx}{a^4} \right)^{-1}. \]

(17)
Substituting in (13), the whole system reduces to

\[ \frac{\partial c}{\partial x} = -\lambda c a^3 \int_0^1 \frac{dx}{a^4}, \quad \frac{\partial a}{\partial t} = -c, \quad \lambda = \frac{8\Lambda \mu D^2}{P_0 B}, \]

(18)
with

\[ c(0, t) = 1, \quad a(x, 0) = a_0(x) < 1. \]

(19)
2.1.2 Specified flux case

In this section we briefly outline how the model changes when the flux through the system, rather than the pressure drop, is specified. The original model (2)–(9) still holds, but now \( P_0 \) in (2) must be considered a function of time, \( P_0(T) \), while equation (3) integrates directly to give

\[
\pi A^2 U_p = Q_p, \tag{20}
\]

where \( Q_p \) is the constant flux per pore. We nondimensionalize the model using the same scalings as in §2.1.1 above, except for

\[
P = \frac{8 \mu D Q_p}{\pi B^4} p, \quad (U, U_p) = \frac{Q_p}{4B^2}(1, u_p). \tag{21}
\]

The resulting model is easily reduced to:

\[
\frac{\partial c}{\partial x} = -\tilde{\lambda} c a^2, \quad \frac{\partial a}{\partial t} = -c, \quad \tilde{\lambda} = \frac{\pi A B^3 D}{Q_p}, \tag{22}
\]

with Darcy pressure \( p \) within the membrane given by

\[
p = \int_x^1 \frac{dx'}{a^4}. \tag{23}
\]

In particular, this last expression allows the pressure \( p(0, t) \) at the membrane inlet (the dimensionless pressure drop in this constant flux case) to be evaluated.

2.2 Model refinement: Pore blocking by sieving

So far, our model has assumed that membrane fouling occurs only due to deposition of particles on the wall of the pores (particle adsorption), at a rate proportional to both the local particle concentration, and to the available wall circumference (equation (8)). This model may be sufficient for feed solutions that contain only particles smaller than pores, but for feed solutions that contain also larger particles in suspension it may be appropriate to account for pore blocking by sieving. In this section we extend our former model (11)–(15) to account for such pore blocking by large particles, which are too large to pass through membrane pores and thus deposit on the membrane upstream surface at a pore entrance. In order to do this, we introduce an additional dependent variable \( N(t) \), the number of unblocked pores per unit membrane area. A reasonable model might be that \( N \) decreases at a rate proportional to the flux through the membrane and to the number of unblocked pores (since a larger flux is associated with a larger carried number of particles; and only open pores can be blocked in this way). With notation as above we therefore propose

\[
\frac{dN(T)}{dT} = -\gamma N(T) U(0, T), \tag{24}
\]

for some constant \( \gamma \), with the initial number of unblocked pores also specified,

\[
N(0) = N_0 = 1/(4B^2). \tag{25}
\]

The blocking of an open pore by a large particle is associated with an additional resistance. When a pore is blocked by this mechanism, we assume its resistance increases by some fixed amount \( \rho_b \).
Adding this resistance “in series” with that of the open pore, we obtain the modified Darcy model replacing Eq. (4),

\[ U = -\frac{\partial P}{\partial X} \left( \frac{N_0 - N}{\frac{8\mu}{\pi A^2} + \rho_b} + \frac{N}{\frac{8\mu}{\pi A^2}} \right). \]  

(26)

Bearing in mind that \( N_0 = 1/4B^2 \), note that Eqs. (26) and (4) are equivalent at \( t = 0 \) (the unblocked system).

### 2.2.1 Specified pressure drop

We nondimensionalize the modified Darcy model comprising (2), (3), (5)–(9), (24)–(26), using the scalings (10) except

\[ (U, U_p) = \frac{\pi B^4 N_0 P_0}{8\mu D}(u, u_p), \quad N = N_0 n. \]  

(27)

The system reduces to:

\[ p = u \int_x^1 \frac{dx'}{a^4(\frac{1-n}{1+r_b a^4} + n)}, \quad u = \left( \int_0^1 \frac{dx'}{a^4(\frac{1-n}{1+r_b a^4} + n)} \right)^{-1}, \quad u_p = 4 \left( \pi a^2 \int_0^1 \frac{dx'}{a^4(\frac{1-n}{1+r_b a^4} + n)} \right)^{-1} \]  

(28)

with \( r_b = \pi \rho_b B^4/(8\mu) \), and

\[ \frac{dn}{dt} = -\Gamma un, \quad \frac{\partial c}{\partial x} = -\hat{\lambda}ca^3, \quad \frac{\partial a}{\partial t} = -c, \quad \hat{\lambda} = \frac{2\Lambda \mu D^2}{P_0 N_0 B^3}, \]  

(29)

with \( \Gamma = \pi \gamma B^5 N_0 P_0/(8\mu D\Lambda\alpha C_0) \), and

\[ c(0, t) = 1, \quad a(x, 0) = a_0(x) < 1. \]  

(30)

### 2.2.2 Specified flux

Similar to §2.1.2, we are also interested in how pressure changes when the flux through the system, rather than pressure drop, is specified for the modified model. Equation (20) still holds, where \( Q_p \) is the constant flux per pore. We nondimensionalize the model using the same scalings as in §2.2.1 above, except

\[ P = \frac{2\mu D Q_p}{\pi B^6 N_0^2}, \quad (U, U_p) = \frac{Q_p}{4B^2}(1, u_p). \]  

(31)

The resulting model is easily reduced to:

\[ \frac{dn}{dt} = -\hat{\Gamma} n, \quad \hat{\Gamma} = \frac{\gamma Q_p}{4\Lambda \alpha C_0 B}, \quad \frac{\partial c}{\partial x} = -\hat{\lambda}ca^3, \quad \frac{\partial a}{\partial t} = -c, \quad \hat{\lambda} = \frac{\pi AB^3 D}{Q_p}, \]  

(32)

with modified Darcy pressure \( p \) within the membrane given by

\[ p = \int_x^1 \frac{dx'}{a^4(\frac{1-n}{1+r_b a^4} + n)}. \]  

(33)
2.3 Model Simulations

In this section we present some sample simulations of the models presented in §§2.1.1, 2.1.2 and §§2.2.1, 2.2.2, showing how results depend on the pore characteristics (shape and size) and on the deposition parameter \( \hat{\lambda} \) (or \( \hat{\lambda} \)). We present results for several different initial pore shapes \( a_0(x) < 1 \) (with the same \( x \)-average, \( \int_0^1 a_0 dx \)); and for different values of the deposition parameters. Additionally, for the constant pressure drop case we also give characteristic plots of flux versus throughput (a common experimental characterization of membrane function), and for the constant flux case we provide plots of pressure drop versus throughput.

2.3.1 Constant pressure drop simulations

Figure 3 shows results for simulating the basic Darcy (adsorption only, no pore blocking by large particles, §2.1.1) for the initial pore profiles

\[
\begin{align*}
  a(x,0) &= \begin{cases} 
  a_1(x,0) = 0.9, \\
  a_2(x,0) = 0.16x + 0.82, \\
  a_3(x,0) = 0.98 - 0.16x, \\
  a_4(x,0) = 0.87 + 0.39(x - 0.5)^2, \\
  a_5(x,0) = 0.93 - 0.33(x - 0.5)^2 
\end{cases}
\end{align*}
\]

all of which average to 0.9, with \( \hat{\lambda} = 1 \), spatial step \( \Delta x = .002 \) and time step \( \Delta t = .002 \). The average pore radius of 0.9 corresponds to a membrane of void fraction \( \phi = \pi(0.9)^2/4 \approx 0.64 \).

Figures 3(a)-(e) show the pore radius for each of these initial profiles at various times throughout the evolution, demonstrating the effect of adsorptive pore-blocking. The most striking feature of these plots is that pore closure (and thus cessation of filtration) always occurs first at the upstream membrane surface, even for pores that are initially widest on that side. A commonly-used experimental characterization of membrane filtration is to plot a graph of flux through the membrane at any given time, versus the total volume of filtrate processed at that time; the so-called flux-throughput graph for the membrane. We plot the dimensionless version of these curves for each of the five pore profiles in Figure 3(f). This graph demonstrates that, although all pore profiles have the same average value, they lead to differences in membrane performance. In particular, membranes whose pores are widest on the upstream side lead to a better performance overall, with more volume processed under the same conditions. The membrane with worst performance is that whose pores are initially narrowest on the upstream side, with rapid pore closure (pore profile \( a_2(x) \) in (34)).

Figure 4 shows the analogous results for the modified Darcy model of §2.2.1 that also includes the effect of pore blocking by large particles. The same initial pore radii are chosen, and the graphs of pore radius variation in time, and total flux versus throughput, are shown with parameters \( \hat{\lambda} = 1, \Gamma = 10 \) and \( r_b = 2 \). The time and spatial steps were as above. The evolution of the pore profiles is quite similar to that in the non-blocking case shown in Fig. 3, with pore closure again always occurring first at the upstream side of the membrane regardless of the initial pore shape. The characteristic flux-throughput curves are now distinctly different in shape however, pointing not only to a system with more total resistance (evidenced by the smaller total throughput at total blocking time), but one whose behavior during the filtration is qualitatively different – the flux-throughput curves for the system of Fig. 3 are all convex, while in Fig. 4 the curves are initially concave, becoming convex only as total system blockage is approached. This change in curvature is indicative of the different blocking regimes: in the early stages the pore-blocking is
the dominant mechanism responsible for the decrease in flux, while in the latter stages adsorptive blocking dominates (at least for the choice of parameters used here).

### 2.3.2 Constant flux simulations

We now present simulations for the case where the total flux through the system, rather than the pressure drop across it, is specified. Figure 5 shows results for both Darcy models, with and without the pore blocking by sieving of large particles (§§2.1.2, 2.2.2) for the same initial pore profiles (34), with spatial and time steps as before, and $\lambda = 1$. Unlike in the constant pressure simulations of §2.3.1 the pore profile evolution is now indistinguishable for the two models, hence figures 5 (a)-(e) are the same for the two models. Figure 5(f) shows the pressure drop versus throughput for each of those pore profiles, for the two models: here, as before, the results for the two blocking models differ.

The results differ quite significantly from those for the constant pressure case. In contrast to those simulations, the pore radius evolution is now much more uniform along the pore length. There is still a tendency for pore closure to happen first at the upstream end of the pores (this happens in four of the five cases considered), but this is no longer inevitable. The pore of linear decreasing radius (Fig. 5(c)) evolves to a state of almost uniform radius, and closes very nearly uniformly (though closure does appear to happen marginally sooner at the upstream end $x = 0$). The concave-up parabolic pore profile actually closes up first at an interior point (Fig. 5(d)).

Since the total flux through the system is held constant the flux-throughput graph gives no characterization of the system in these simulations, hence we instead plot how the pressure drop rises over time as blocking occurs in order to maintain the specified flow rate (Fig. 5(e)). The two models give rise to qualitatively similar behavior; as anticipated, the main difference is that the model with additional blockage by large particles is associated with higher pressures throughout, due to the larger total resistance. As with the constant pressure simulations, the best overall performance (in terms of efficiency) is provided by the pores of monotone decreasing radius (profile $a_3(x)$ in (34)), and the worst by pores of monotone increasing radius profile (profile $a_2(x)$).

### 2.4 Conclusions for the Darcy flow model

Figures 3 and 4 show that for the case of specified pressure drop case, no matter how the initial pore profiles are chosen, the highest deposition of particles occurs at the upstream side ($x = 0$) of the filter. This is especially true for the model considering blocking by large particles. Although this additional blockage mode decreases overall efficiency in the sense of requiring more energy to process the same volume of feed solution, it may be that the large particles improve the overall separation efficiency, in the sense that for these simulations we have less deposition at the end of pore $x = 1$, indicating that fewer particles have the chance to escape the filter. In other words, for the case which considers sieving by large particles, most of the particles deposit in the first 30% of the pore depth; as figure 4 shows, there is almost no deposition at the pore exit. This is due to the fact that the large particles themselves increase the system resistance (the factor $\rho_b$ in equation (26)).

These observations exemplify the tradeoffs that must often be made in micro filtration: finer separation is generally associated with larger energy needs: the figures 3(f) and 4(f) show the total filtered fluid volume for the dual-blocking-modes case is less than for the simple case.

Needless to say, the choice of initial pore profile strongly affects the fouling mechanism. Since the pore blocking occurs primarily at the upstream side of the filter $x = 0$ for the specified pressure
Figure 3: Constant pressure drop case, Darcy model without blocking by large particles: The pore radius at several different times at different final blocking times ($t_f$) (indicated in the legend) for different initial pore radius profiles, (a) $a_1(x,0) = .9$, (b) $a_2(x,0) = 0.16x + 0.82$, (c) $a_3(x,0) = 0.98 - 0.16x$, (d) $a_4(x,0) = 0.87 + 0.39(x - 0.5)^2$, (e) $a_5(x,0) = 0.93 - 0.33(x - 0.5)^2$. (f) Total flux vs throughput for those initial pore radius profiles.
Figure 4: Constant pressure drop case, Darcy model with blocking by large particles: The pore radius at several different times at different final blocking times ($t_f$) (indicated in the legend) for different initial pore radius profiles, (a) $a_1(x,0) = .9$, (b) $a_2(x,0) = 0.16x + 0.82$, (c) $a_3(x,0) = 0.98 - 0.16x$, (d) $a_4(x,0) = 0.87 + .39(x - 0.5)^2$, (e) $a_5(x,0) = 0.93 - 0.33(x - 0.5)^2$. (f) Total flux vs throughput for those initial pore radius profiles.
Figure 5: Constant flux case, Darcy model with/without blocking by large particles: The pore radius at several different times at different final blocking times ($t_f$) (indicated in the legend) for different initial pore radius profiles, (a) $a_1(x,0) = .9$, (b) $a_2(x,0) = 0.16x + 0.82$, (c) $a_3(x,0) = 0.98 - 0.16x$, (d) $a_4(x,0) = 0.87 + .39(x - 0.5)^2$, (e) $a_5(x,0) = 0.93 - 0.33(x - 0.5)^2$. (f) Pressure drop vs throughput for those initial pore radius profiles.
drop case, blocking of the pores which have larger radius at this end takes more time (and vice versa). In general our results suggest that pore size gradations from large on the upstream side to small on the downstream side will produce better outcomes in terms of efficiency.

Figure 5(a-e) shows that when flux, rather than pressure drop, is specified, pore closure may happen in the middle of the membrane rather than at $x = 0$, but still in most of the cases we have blocking at $x = 0$. In this case, both models (blocking with and without large particles) have identical pore profile evolution, since the forced pressure on the top which maintains the flux during the fouling process, forces the fluid to pass through pores at the same rate, regardless of whether large particles block the pores or not. Mathematically speaking, the governing equations for pore radius and particle concentration, equations (22) and (32), for both cases with/without blocking by large particles, are the same. The only difference between these two cases, according to figure 5, is that for the blocking case we need to have more pressure in order to satisfy the constant flux condition.

3 Particle capture by flow around structures within membrane: CFD Modeling

The Workshop participants also considered alternative flow scenarios, more descriptive of a node-fibril membrane microstructure of the type seen in Fig. 1 (c),(d). The notation used in the description below should be considered independently of that in §2.

3.1 Methods

We simulate the capture of particles in a flow according to the following model. Consider the geometry shown in Fig. 6. Fluid flows in across the boundary on the left side with a constant velocity $U$, and continues around a long fiber with ellipsoidal cross-section. The flow itself is modeled using the incompressible Navier-Stokes equations:

\[
\frac{\partial \mathbf{u}^*}{\partial t^*} + (\mathbf{u}^* \cdot \nabla^*) \mathbf{u}^* = -\nabla^* p^* + \nu \nabla^{*2} \mathbf{u}^* \\
\nabla^* \cdot \mathbf{u}^* = 0.
\]

Here, $\mathbf{u}^* = (u^*, v^*)$ is the fluid velocity, $p^*$ is the pressure, $\nu$ is the kinematic viscosity, and asterisks indicate that the variables are dimensional. The ellipsoidal fiber is treated as a long, continuous distribution of charges with strength $Q$ per unit length. If a particle with charge $q$ approaches the
electric field generated by the fiber, its drift velocity towards the fiber can be modeled according to the following expression \[4\]:

\[ V_{d}^* = \frac{Qq}{6\pi^2\epsilon_0\mu d_p r^*} \]  

where \(\epsilon_0\) is the permittivity of free space, \(\mu\) is the dynamic viscosity, \(d_p\) is the particle radius, and \(r^*\) is the distance from the particle to the center of the fiber.

Introducing length scale \(l_c\), time scale \(t_c\), and mass scale \(M_c\), we define the following dimensionless variables:

\[ t = \frac{t^*}{t_c}, \quad (x, y) = \left(\frac{x^*, y^*}{l_c}\right), \quad (u, v) = \left(\frac{u^*, v^*}{t_c}\right), \quad p = \frac{p^* t_c^2}{l_c^2} \]

Hence the dimensionless Navier-Stokes equations are

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p + \frac{1}{Re} \nabla^2 u \quad (38)
\]

\[
\nabla \cdot u = 0 \quad (39)
\]

where \(Re = l_c^2 / t_c \nu\) is the Reynolds number of the flow. Eq. (37) becomes

\[ V_d = E \frac{r}{r^*} \]  

where \(E = \frac{Qq l_c}{6\pi^2\epsilon_0\mu d_p l_c^2}\) is now the single parameter characterizing the strength of the interaction between the fiber and the particle in the flow.

We choose the following scales, provided by the Pall Corp: \(l_c = 1\mu m\), \(t_c = 18\mu s\), \(M_c = 10^{-15}kg\). With these scales, \(a \approx b \approx 0.2\) (for a circular cylinder), \(U = 0.1\), and \(Re = 0.1\). Our computational domain, unless otherwise noted, consists of a unit square \(D = [0, 1] \times [0, 1]\). The boundary conditions on all variables on all boundaries is homogeneous Neumann, with the exception of the following conditions:

- \(u|_{x=0} = U\)
- \(p|_{x=1} = 0\)
- \(\frac{\partial u}{\partial x}|_{x=1} = 0\)
- \((u, v) = 0\) on the surface of the fiber.

The system Eqs. (38)-(39) is solved using an open source Navier-Stokes solver [9–11]. We couple this to the motion of the charged particle according to the following expression:

\[
\frac{d\xi}{dt} = u + V_D \]  

where \(\xi(t)\) is the particle location. The initial location of the particle is given by

\[ \xi(0) = (0, y_i) \]

so that the particle always enters from the left side, but with variable \(y\) coordinate. Eq. (41) is solved by fourth order Runge-Kutta method; the values of \(u\) are interpolated from the cell centered values obtained from the Navier-Stokes solver. Finally, a particle is considered captured if the distance between the particle center and the surface of the fiber drops below a certain threshold; no account of particle adhesion to the fiber is built into the model.
3.2 Results

Figure 7 shows computational results for circular fibers with radius of 0.2. Particle trajectories are shown by red curves. All particles enter from the left side of the domain, and move unidirectionally along these trajectories. Figure 7(a) demonstrates that for large $E$, roughly one-tenth the strength of the incoming fluid velocity, the particles are captured by the fiber over a large capture radius, even reversing direction and becoming captured after they have passed by the fiber. As we would expect, a smaller capture radius is observed for a smaller $E$ in Fig. 7(b). We show a similar result for fibers with an elliptical cross-section with $a = 0.2$ and $b = 0.1$ in Fig. 8.

We show the flow around multiple fibers with circular cross-sections in Fig. 9. Here, the computational domain $D = [0, 2] \times [0, 1]$ contains six fibers with radii $a = b = 0.2$ with random center locations. The competing attractions of multiple fibers to the particles have a canceling effect, so that most particles move completely past the fibers without being captured.

4 Particle capture by flow around structures within membrane: Analytical approach

In addition to the CFD approach described above, the Workshop participants also considered an analytical approach to the problem of particle capture by nodes or fibrils. In an attempt to characterize the process of particle deposition within the membrane a set of model problems was considered. Assuming a membrane to be composed of an interconnected set of simple objects such as spheres and/or cylinders, we considered the flow of small particles, carried by the feed solution, around such obstacles. Equations describing the concentration of a population of particles, undergoing advection, diffusion and electrostatic interaction with the obstacle, were written down and analyzed. Dimensional analysis revealed that diffusion is dominated by advection and electrostatic forcing over most of the flow domain, except in some small region around the obstacle (small compared with the obstacle diameter but perhaps large compared with the particle size). The model for particle
transport was solved for the simplest canonical obstacle geometry (a spherical inclusion) in the case where diffusion is neglected entirely. In this case an expression can be obtained, in terms of simple model parameters relating to the membrane internal structure, for the proportion of particles that are captured by the obstacle. If one considers the membrane to be composed of a periodic lattice of spherical inclusions (for example) such considerations enable one to predict the proportion of particles captured by a membrane consisting of a given number of layers. These results are not described in detail in this report.

5 Considerations of fractal structure of membranes

A search of the relevant literature revealed that other authors (e.g. Yu & Lee [12]) have considered porous media with highly complex internal structure, and have written down explicit expressions for membrane characteristics such as permeability, tortuosity, etc., in terms of the fractal dimension of the membrane (which may itself be calculated from detailed SEM membrane images). Such geometrical considerations can provide a useful framework to characterize clean membranes. Clean
membrane characteristics are needed as input to the type of fouling models described in §§2, 3.

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References


