Effects of membrane morphology on separation efficiency

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Devise a common mathematical description of membrane morphology which
- Distinguishes common membrane types
- Connects to separation and fouling performance
Darcy flow modeling $\text{Re} \ll 1$

- Darcy model gives $u = -\frac{k(x,t)}{\mu} \frac{\partial p}{\partial x}(x, t)$, where by continuity

$$(k(x, t)p_x(x, t))_x = 0$$

with pressure drop or flux across membrane specified.

- Consider simple sub-models in which $k(x, t)$ may be written explicitly in terms of membrane characteristics.
Simple tube model: schematic
Simple tube model: Governing equations

- $u$: superficial (Darcy) velocity; $u_p$: pore velocity; $a(x, t)$: pore radius; $c(x, t)$: particle concentration; $b$: size of period box.

\[
\begin{align*}
    u &= -\frac{a^2}{8\mu} \frac{\partial p}{\partial x} \\
    ub^2 &= \pi a^2 u_p & \text{Relation between superficial and pore velocity} \\
    \frac{\partial}{\partial x} (u_pa^2) &= 0 & \text{Continuity} \\
    u_p \frac{\partial c}{\partial x} &= -\lambda ca & \text{Particle advection & deposition} \\
    \frac{\partial a}{\partial t} &= -\lambda \alpha c & \text{Pore shrinkage}
\end{align*}
\]

- $\lambda$ is the capture efficiency.
- Constant pressure drop or constant flux.
Simulations: $P_0$ fixed, asymmetric membrane

$$a(x, t = 0) = -0.1 \sin(2\pi x) + 1$$
Simulation: $P_0$ fixed, asymmetric membrane

Radius of the cross section of the pore at "almost" blockage time

for $a(x, t = 0) = -0.1 \sin(2\pi x) + 1$
Simulations: Flux fixed, asymmetric membrane

\[ a(x, t = 0) = -0.1x + 1 \]
Modeling the microscale structure

Model the microscale in order to determine the capture efficiency.
Consider a simple filter made only of charged spheres
Assume the filtrate follows Stokes flow around the spheres
The particles in the fluid are pushed by the flow, but are also pulled by the electrostatic force toward the sphere. This leads to the equation (for a sphere with radius 1)

$$- \left( \frac{3x^2}{2} \cos \theta + E \right) C_x + \frac{3x}{2} \sin \theta C_\theta = 0$$

Estimate the permeability by finding the streamtube in which particles are pulled toward the sphere.
The Stokes Flow linearized close to a sphere is given by

\[ q_r = -\cos \theta \frac{3x^2}{2}, \quad q_\theta = \sin \theta \frac{3x}{2} \]
If the particle has negligible radius, we find a separatrix solution which is the boundary of the stream tube

\[ x^*(\theta) = \sqrt{\frac{4e \cos \theta + 4E}{3 \sin^2 \theta}} \]

And the streamtube has a radius \( r = 2 \sqrt{\frac{2E}{3}} \) far away from the sphere.
A Microscale Approach

When incorporating a finite particle radius \( d \), the separatrix solution is

\[
x^*(\theta) = \sqrt{\frac{4E \cos \theta + 3d^2 + \frac{4E^2}{3d^2}}{3 \sin^2 \theta}}
\]

And this streamtube has a radius \( r = \sqrt{\frac{4E+3d^2+\frac{4E^2}{3d^2}}{3}} \) far away from the sphere.
Navier-Stokes Model

We developed a program to simulate particle capture as follows:

1. Simulate the full Navier-Stokes equations for the flow field $\mathbf{u}$ around an (in principle) arbitrary solid geometry (the filter):

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \nu \nabla^2 \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0$$

Solved using a finite volume method (implemented in Gerris) with $\nu = 10$.

2. Particle paths follow the flow field subject to a perturbation by the electrical forcing:

$$d_t \mathbf{x} = \mathbf{u} + V_D$$
Geometry and Nondimensionalization

We simulate the capture due to a filament with an ellipsoidal shape with an electrical charge density $\lambda$.

The deflection of the particles toward a line of charges is given by

$$V_D = \frac{\lambda q}{6\pi^2 \varepsilon_0 \mu_d p r}$$

$T = 18\mu s, \ L = 1\mu m, \ Q = 1e, \ M = 10^{-15} kg$

$\Rightarrow \ a, b \approx 0.2 \quad U = 0.1 \quad V_D = V/r$
Circle

(a) \( V_d = 0.001 \)

(b) \( V_d = 0.01 \)
Ellipse

(c) $V_d = 0.001$

(d) $V_d = 0.01$
Ellipse

$V_d = 0.001$

$V_d = 0.01$
Flow in other geometries
Prefractal analysis - porous membrane

Permeability of porous membrane (Yu & Lee, 2002):

\[ k = G \frac{L_0^{1-D_T}}{A} \frac{D_f}{3 + D_T - D_f} \lambda_{\text{max}}^{3+D_T} \]

- \( G, L_0, A \) - geometric factors
- \( D_T \) - tortuosity fractal dimension, \( 1 < D_T < 2 \)
- \( D_f \) - pore area fractal dimension, \( 1 < D_f < 2 \)
- \( \lambda_{\text{max}} \) - maximum pore size
Permeability of cake layer (Meng et al., 2005):

\[ k = \frac{G}{g^2} C_0 \frac{1}{A_t} \frac{2 - D_s}{3 - D_s} a_{\text{max}}^{3-D_s} \]

- \( G, g, C_0, A_t \) - geometric factors
- \( D_s \) - pore area fractal dimension, \( 1 < D_s < 2 \)
- \( a_{\text{max}} \) - maximum area of pores
We have developed a Darcy model of flow through an asymmetric membrane that includes fouling with a spatial and time dependent permeability with a specific pore model.

We have characterized the capture of particles travelling near an obstacle due to contact and electrostatic attraction, and classified the behavior based on the importance of electric attraction.

Navier-Stokes simulations of the flow past an arbitrary geometry with particles which are captured due to contact and electrostatic attraction.
Acknowledgements

Thank you for your attention and our sponsors for making this possible!

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Extension: Include pore-blocking by large particles

- In addition to blocking by adsorption, allow also large particles to block pores from above. Introduce additional variable $N(t)$: number of unblocked pores per unit membrane area.
- Assume pores block at a rate dependent on the flux $u$:
  \[
  \frac{dN}{dt} = -\gamma u, \quad N(0) = N_0.
  \]
- When a pore is blocked by this mechanism, assume its resistance increases by some fixed amount $\rho_b$. Adding this resistance “in series” to the membrane resistance due to the narrowing pores, obtain modified Darcy model
  \[
  u = -\frac{\partial p}{\partial x} \left( \frac{N_0 - N}{\frac{8\mu}{\pi a^4} + \rho_b} + \frac{N}{\frac{8\mu}{\pi a^4}} \right)
  \]
- These equations augment previous model (simulations to be done).