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Incorporating pore blocking, cake filtration, and EPS production in a model for constant pressure bacterial fouling during dead-end microfiltration

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ABSTRACT

Microfiltration is used in a wide range of municipal and industrial settings to remove particulate matter including pathogenic microorganisms such as bacteria and protozoa. As more water is filtered at constant pressure, the accumulation of retained particles on the membrane decreases the filtration rate; a process commonly referred to as fouling. Mathematical treatment of flux decline has proved to be a useful tool in diagnosing filtration data even though the mathematical underpinnings are not completely understood. In particular, little is known about the transition between fouling phenomena (e.g. pore blocking to cake filtration). Moreover, less is known about the effect of extracellular polymeric substances (EPS) production by bacteria when they accumulate on a membrane over extended durations. In this manuscript, we develop a novel approach to model bacterial microfiltration by considering the effects of both differential binding and exopolymer production. Spatial gradients in bacteria concentrations initially occur due to the non-uniform membrane surface porosity and differential deposition caused by the stochastic nature of microorganism adhesion. These heterogeneities in bacterial deposition and associated pore blocking result in variable secretion of extracellular polymers. Long-term fouling is quantified as the cumulative resistance posed by both bound bacteria and EPS. We compare numerical simulations quantitatively and qualitatively to previously published experimental data and investigate variations of microbial deposition patterns across the membrane. We find substantial agreement between the model and experimental observations. We are also able to conclude that fluid dynamics must be important if the dominant variability is in the membrane structure, rather than in bacterial adhesion. However, variation in bacterial adhesion alone can also induce substantial spatial heterogeneity.

1. Introduction

During constant pressure dead-end filtration the build up of filtered particulate matter impedes the performance of the filter by blocking the pores. It is widely recognized that the effect of preblocking on the filtration rate depends on the size and density of the particle load as well as the volume of fluid that has been filtered [1–5]. Currently there are four empirical models of blocking that account for different regimes of the experiments [6]. If the particulates are small relative to the pore size, and the volume that has been filtered is small a 'standard' blocking law can be derived. If the particles are larger than the pores a similar 'complete' blocking law has been proposed. After some volume has been filtered and there are particles bound to the filter an intermediate blocking law is applicable as long as the probability that an incoming particle attaches to the filter is equal to the probability that it attaches to a previously deposited particle. Finally, when nearly the entire filter has been coated with particles the decline in the flux is largely due to frictional (viscous) losses within the surface deposit or cake and can be represented through a cake blocking law.

Each of these regimes can be seen in a wide variety of dead-end filtration experiments, where predictions from different blocking laws agree with experimental measurements at different times. Because the forms of the four blocking laws are conceptually related as,

$$\frac{d^2t}{dV^2} = k\left(\frac{dt}{dV}\right)^n \quad (1)$$

one could try and estimate the parameters κ and n for a particular experimental design and use the appropriate blocking-law model to predict the filtration performance. More generally one could even assume that κ and n were not constant; however, it is not at all clear how to predict which model to use without extensive experimental observation. Therefore, it would be helpful to develop

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a model that handled the transition between various regimes (clean filter, partially fouled filter and cake-fouled filter).

There has been significant progress along these lines already [3,7,8]. One of the extensions assumes that there are two components that influence the flux decline during protein filtration. One part is introduced by the suspended aggregates directly blocking the pores, while the other part is due to proteins depositing on each other. Typically, the authors assume that the total flow rate through the filter is the sum of the flow rate through the open and blocked pores, where each flow rate is proportional to the product of the open (blocked) area and the ratio of the pressure to the open resistance [3]. There is an additional resistance that differentiates between the resistance of flow through the open and blocked regions. In [3], this resistance is ascribed to the protein deposition. By using conventional relationships between flow rate, flux and resistance a conceptual model was derived that compared favorably with experimental measurements. Other investigators have also characterized pore blocking and cake formation (e.g. [9–11]).

This current investigation considers two aspects of filtration that were not considered in [3]. The first is concerned with the irregular spatial deposition patterns that have been observed during dead-end filtration [12,13]. In a previous investigation the interaction between the fouling of the filter and the fluid dynamics that transport suspended particles to the membrane was shown to induce spatial patterns [14]. Here, we consider a different framework. Rather than considering the explicit fluid dynamics, we consider the possibility that differential attachment might be due to stochastic adhesion. We introduce two different particular mechanisms. The first is related to the spatial variability in surface porosity inherent to all commercially available membranes as in [14], although the fluid dynamics are not addressed. Rather, we assume that there are variations in the likelihood of attachment or irreversible deposition, that depends on the initial porosity of the membrane. A second, different mechanism assumes that individual attachment is a stochastic event, with a probability that changes independent of time. More details regarding these mechanisms are given below, but we note that the first can be conceptually related to the previous investigation if we assume that bacteria are more likely to attach in regions of high porosity. We are neglecting the effect this has on the transport of the bacteria.

The second extension that we consider is the effect of production of extracellular polymeric substances (EPS) by the bacteria. It is known that when bacteria attach to a surface, or are surrounded by high numbers of bacteria, they tend to begin producing (EPS), which are largely comprised of proteins, polysaccharides, lipids, humic substances, and nucleic acids [15,17]. EPS production presumably affects the water flux in a different manner than the protein deposition in [3,18] since it is coupled with the particle (bacterial) concentration on the filter. We show that the EPS production can account for the transition from the intermediate blocking behavior to the cake-blocking behavior that is typically observed. Operationally, several studies have linked EPS concentrations with fouling in low-pressure membrane systems (e.g. [19]). However, the role of EPS on cake resistance has not yet been quantitatively incorporated in modeling flux decline during bacterial filtration (e.g. [20,21]) even though experimental evidence has demonstrated that it is a major component of fouling in such systems, especially during long-term operation [22,23].

In the next sections we describe two different models to understand the behavior of dead-end filtration. The first is a macroscopic model, that neglects any spatial variations and focuses on the EPS production and the transition between different filtration regimes. We show that a simple, phenomenological treatment of EPS production explains the transition from pore blocking to cake filtration quite well. The macroscale model motivates a microscale model that considers the spatial variation and stochastic differences in attachment. Connecting the two models yields a single overall model that is tractable and reflects experimental results over a range of parameters. This is demonstrated in several numerical simulations described in Section 3.

Table 1
List of parameters and values used in the simulations.

Mathematical notation	Description
α	Areal coverage fraction
γ	EPS sensitivity
κ	Bacterial deposition rate
κ_1	EPS production rate
λ	Darcy constant (ratio of pressure drop to viscosity)
μ_a	Maximum bacterial resistance
μ	Viscosity
A_{open}	Open fraction of membrane
B_b	Concentration of bound bacteria
B^*	Reference bacterial density
E	EPS density
J	Flux
K	Bacterial resistance saturation constant
P	Pressure
R_m	Clean membrane resistance
R_a	Bacterial specific resistance
R_e	EPS specific resistance
t	Time
$\mathbf{U}$	Velocity field
V	Volume

2. Mathematical model

We begin with a macroscale model representing the flow and free bacterial density dynamics. We argue that on the macroscopic scale, the fluid dynamics are trivial. This allows us to focus on the other components of the model. Although the argument that the fluid dynamics are negligible for the macroscopic model, this is not the case for the microscale model in general. However, the macroscale model motivates a simplified microscale model, where the fluid motion is neglected while typical blocking curves are recovered. This suggests that the two mechanisms that introduce spatial variations (fluid interactions and stochastic binding) may be independent. For the current investigation, we will not consider local fluid variations leaving the combined mechanisms for later investigation. We compile a list of mathematical notation in Table 1.

2.1. Macroscale model

On the macroscale, the filtration model consists of equations governing the fluid velocity and the particulate matter (bacteria). In an earlier investigation a model was proposed that focused on how inhomogeneous fouling of the filter could be reinforced by the fluid dynamics. Here we propose a similar model that differs by neglecting the heterogeneity of the flow on the macroscale. This macroscale model suggests forms for a detailed study of the particle distribution on the membrane so that we are able to address variations that are inherent in the particles and membrane.

Based on typical length and velocity scales, the fluid dynamics are well described by incompressible Stokes equations,

$$\mu \Delta \mathbf{U} = \nabla P \tag{2}$$

$$\nabla \cdot \mathbf{U} = 0 \tag{3}$$

where $\mathbf{U} = (U^x, U^y)$ denotes the fluid velocity perpendicular (x) and parallel (y) to the filter. and μ is the fluid viscosity.

If the inflow and outflow are assumed to have no y-component, there is no symmetry breaking, so these equations can be reduced to a one dimensional model. Incompressibility (Eq. (3)) requires that the flow be constant in space. The fluid velocity attained for a constant pressure drop is a constant in space. It depends on time