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A network-based approach to interpreting pore blockage and cake filtration during membrane fouling

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ABSTRACT

The efficiency of membrane-based separations is limited by various fouling phenomena, which necessitates a mechanistic understanding in order to improve such processes. This study proposes a network-based approach, in which the membrane is discretized and each particle is individually monitored, to explore the underlying fouling mechanisms leading to pore blockage and cake growth during a membrane filtration process. In particular, the network-based approach provides more spatial resolution than the continuum approach, thereby gives a more in-depth insight into membrane fouling. The network model developed involves the construction of a two-dimensional (2D) network of pores to represent the membrane, a series of probabilistic criteria to describe the fate of each individual particle, and finally a protocol for evaluating the fouling during either a constant flux or constant TMP (transmembrane pressure) filtration. Three fouling parameters can be obtained to characterize the fouling behavior, namely, the probabilistic factor for deposition in the dead zone (β), the initial cake resistance (R_{c0}), and the specific cake resistance with respect to cake thickness (R'_c), by best-fitting the experimental flux-decline data to the network model. The capability of the network model to account for the topological and stochastic aspects of a fouling process provides for a more mechanistic understanding of the complex interactions between the fluid flow, membrane, and foulant particles vis-à-vis a model based on the continuum assumption. Although limited fouling cases were examined in the current study, it is expected that the network model developed here can be readily applied to study more complex phenomena involved in a membrane filtration process (e.g., shear-induced diffusion), and the associated insights would be significantly enhanced when coupled with more advanced fouling characterization techniques (e.g., Optical Coherence Tomography).

1. Introduction

Membrane fouling is a complex phenomenon that involves the interplay between fluid dynamics, foulants, and membrane materials during a membrane filtration process. Developing techniques for effectively mitigating membrane fouling to a great extent relies on an in-depth understanding of the mechanisms that underlies how the overall behavior of the filtration system, such as the variation in the permeation flow rate or trans-membrane pressure (TMP), responds to the dynamics of foulant deposition at multiple scales. Although experimental studies are the most direct way to explore the membrane fouling phenomena, mathematical modeling plays an essential role in interpreting various fouling mechanisms and extracting the intrinsic physics.

As reviewed by Sahimi et al. [1], mathematical models for describing the transport phenomena associated with a porous medium can be classified into continuum and discrete models. The continuum models have been extensively employed to study membrane fouling, including the classical fouling models (namely, the complete pore blockage model [2,3], the intermediate pore blockage model, the cake filtration model [4], and the pore constriction model [5,6]) and lately evolved into models that account for multiple fouling mechanisms, such as the combined fouling model (which coupled not only the complete and intermediate pore blockage model but also the cake filtration model) by Ho and Zydney [5] and the three-mechanism model by Duclos-Orsello et al. [3]. Despite having different focuses on the dominant membrane fouling mechanism, these fouling models are based on the assumption that not only the spatial domains (e.g., the membrane and the fluid channel) but also the velocity and concentration fields can be described by smooth functions. The dynamical processes are described by the

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Nomenclature

A_{nw}	the membrane area to be simulated, m^2
A_u	area of a unit cell, m^2
c_f	the weight concentration of the feed solution, g/L
$\overline{d}_{mp}$	the mean of pore diameter, m
$\overline{d}_p$	average particle diameter, m
d_u	the pore diameter, m
H_w	the height difference of water column, m
J_{mp}	the fluid velocity through a pore, m/s
L_c	the thickness of the cake layer, m
m_p	the deposit mass, kg
N_{du}	the number of the unit cells without pores, -
N_f	the number of particles per unit volume, L^{-1}
N_u	the number of the unit cells, -
$N_{u,\max}$	maximum number of the unit cells, -
N_{up}	number of pores in each unit cell, -
P_b	probability of a particle blocking an open pore, -
P_c	probability of a particle depositing on the particle layer, -
P_d	probability of a particle contacting a unit cell without pores, -
P_i	probability of a particle contacting a unit cell with pores, -
P_m	probability of a particle depositing on the dead zone of the membrane (i.e., region without pore), -
P_u	probability of a particle depositing on a unit cell, -
Δp	pressure drop during filtration, Pa
$Q_m(t_i)$	permeation flow rate measured during the fouling experiment, m^3/s
$\hat{Q}_m(t_i)$	permeation flow rate evaluated at the times corresponding to the sampling points of the fouling experiment, m^3/s
Q_{nw}	permeation flow rate, m^3/s
Q_t	total flowrate, m^3/s
R_c	cake resistance, m^{-1}
R_c'	specific resistance with respect to the cake thickness, m^{-2}
R_{c0}	initial cake resistance, m^{-1}
R_{mp}	hydraulic resistance of the cylindrical pore, m^{-1}
R_{p0}	initial resistance of the deposit, m^{-1}
R'_p	the specific deposit resistance, m/kg
Δt_i	duration of the ith simulation period
V_{up}	the total volume of the particles rejected in the unit cell, m^3
X	randomly generated number between 0 and 1 to compare with probability, -
Y	randomly generated number between 0 and 1 to compare with probability, -
Z	randomly generated number between 0 and 1 to compare with probability, -

Greek symbols

α	pore blockage parameter, m^2/kg
β	probabilistic factor for deposition in the dead zone of the membrane, -
ε_c	porosity of cake layer, -
ε_m	membrane porosity, -
ε_u	porosity of a unit cell, -
ϕ_{ud}	fraction of the unit cells without pores, -
ϕ_{uo}	fraction of the unit cells with pores, -
ρ_p	particle density, kg/m^3
μ	viscosity of the feed solution, Pa s

phenomenological relations [7,8], but the topological aspects of membrane fouling, such as the connectivity of the porous structure and the distribution of the deposits, are ignored owing to mathematical complexities.

Taking advantage of the advancement in computational capacity and algorithms, discrete models are getting more attention in the field of membrane process simulation. Instead of assuming a continuum, a discrete model represents the spatial domain as an array of unit cells and thereby adapts the species conservation law to the individual unit cells. The array of unit cells to represent the membrane topology is referred to as a network. Such network models are developed to accommodate random processes by establishing a series of probabilistic criteria [9], which is key to understanding and simulating membrane fouling as the local fouling behavior is stochastic in nature [10]. A network-based method has been proposed by Li [9] to investigate the effects of membrane asymmetry on membrane fouling, and further extended to account for the concentration polarization within the supporting structure of a forward osmosis (FO) membrane [11]. More recently, Griffiths et al. [12] employed a similar network model to theoretically interpret the flux-decline behavior during membrane fouling. A key advantage of network modeling highlighted by these studies is the much enhanced spatial resolution relative to the continuum model. The ability to account for the local fouling behavior at a scale defined by a unit cell allows for the accounting of the topological and stochastic aspects of a fouling process, and is significant in the understanding of the fouling phenomenon on two counts. Firstly, it offers a tool for correlating the experimental observations from advanced characterization techniques for studying membrane fouling, such as the direct observation through the membrane (DOTM) [13], optical coherence tomography (OCT) [14], and electrochemical impedance spectroscopy (EIS) [15]. Secondly, it provides a highly flexible framework whereby each fouling mechanism can not only be readily extracted for a mechanistic understanding, but also readily combined to simulate practical fouling processes under various operating conditions.

The current study was aimed at developing a systematic approach to analyze membrane fouling via network modeling. In particular, the focus was on interpreting the pore blockage and cake growth on the membrane surface, both of which are categorized as external fouling in the literature [16–18]. The specific objectives in the overarching goal of developing the network model were to (i) determine the numerical stability and sensitivity of the model, (ii) compare the network model developed with the well-established continuum model [5], and (iii) validate the network model with experimental data. Accordingly, the steps taken in constructing the network model were: (1) to construct a two-dimensional (2D) network of pores to approximate a membrane having pores with specific distributions in size and location; (2) to establish a series of probabilistic criteria to describe the fates of each foulant particle; and (3) to develop a protocol for assessing both a constant flux and constant TMP (transmembrane pressure) filtration process.

2. Model development

2.1. Constructing a network

The key basis of a network-based simulation is to approximate the porous structure or membrane with a hypothetical network that has two or three dimensions. Although the proposed method can be readily extended to account for more complicated membrane structures, it is expedient to restrict the current study to membranes having the simplest porous structure, i.e., uniform straight through cylindrical pores, so as to validate the model. Because the thickness of the membrane is very much smaller than the area of the membrane evaluated, a two-dimensional (2D) network can be used to approximate the membrane.