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A two-dimensional mechanistic model for scaling in spiral wound membrane systems

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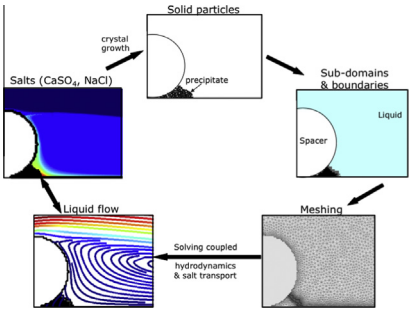
HIGHLIGHTS

- 2-d Model was developed for mineral precipitation in membrane feed channels.
- The model suggests membrane-spacer contact points are prone to scaling.
- Local concentration of solutes and flow conditions are important for precipitation.
- Thermodynamic and kinetic effects govern gypsum precipitation in membrane channels.
- General trends for performance decline are well described by the numerical results.

GRAPHICAL ABSTRACT



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ABSTRACT

A two-dimensional mathematical model integrating fluid flow and solutes mass transport with a particle-based approach for crystal nucleation and growth was developed to study gypsum ($CaSO_4{\cdot}2H_2O$) scaling in membrane feed channels. The model is able to describe the generally observed trends for performance decline due to scaling: permeate flux deterioration when constant pressure is applied and trans-membrane pressure increase when a constant permeate flux is set.

Model results for precipitation in the feed channel show a gradual increase of precipitated gypsum in the axial direction. The zones around spacer-membrane contacts are most prone to scaling even when the feed water is under-saturated. Simulations highlight the importance of both thermodynamic and kinetic effects on gypsum precipitation for various salinities. Despite having the same degree of saturation of the feed water, variable feed stream compositions result in different amounts of precipitate formed. The numerical results suggest that the degree of saturation of feed water (DS_{in}) may not be a reliable indicator for precipitate formation in membrane feed channels.

Results support the need for considering the dynamics of local flow and solute patterns, combined with ionic activity calculations for understanding mineral precipitation in spiral-wound membrane modules used in desalination.

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1. Introduction

Fresh water scarcity in various regions around the world has resulted in an increased use of desalination processes [1], able to convert seawater, brackish water or wastewater effluent into high quality water. Reverse osmosis (RO) and nanofiltration (NF) membrane systems are an essential component for most treatment plants for drinking and industrial water production worldwide. One of the problems with these membrane processes is scaling due to crystallization of sparingly soluble salts [2]. Scaling leads to lower water recovery rates and increased maintenance costs. The use of chemicals to prevent salt precipitation (anti-scalants) in membrane filtration processes increases water production costs and can cause problems with concentrate disposal [3,4]. Additionally, some commonly used anti-scalants have been shown to potentially accelerate microbial biofilm formation [5].

Limited possibilities have been identified so far for in situ scaling studies, e.g., Ultrasonic Time Domain Reflectometry [6–8], visual observations [9,10], and impedance spectroscopy [4]. Monitoring of certain global variables (turbidity, pH, Ca^{2+}, permeate flux) has been suggested to have inadequate sensitivity for detecting early scaling events [4,11]. Most of the times, scaling is only diagnosed during membrane autopsy (by Inductive Coupling Plasma, Scanning Electron Microscopy, gravimetric measurements). Antony et al. [4] provided an overview of currently applied prediction and control techniques for mineral scaling in membrane systems, while highlighting that scaling remains a challenge within the RO industry.

The constraints on experimental scaling studies prevent the comprehensive understanding of the causes and consequences of precipitate formation. Several researchers attempted to improve the knowledge on scaling potential and precipitation in membrane systems by using mathematical models. These models usually estimate concentration profiles at the membrane surface using the film theory, resulting in a spatially averaged concentration polarization (CP). Lee and Lee [12] proposed a lumped model incorporating both bulk and surface nucleation to fit experimental data obtained under various operational conditions for NF membranes. With similar assumptions, Oh et al. [13] described numerically the effect of scaling on flux for stirred and cross-flow RO flow. Although good fitting to particular experimental data was achieved, these models may be too simplified, as it is well acknowledged that solute concentrations change within a membrane module [14].

Bhattacharjee and Johnston [15] presented a model including axial concentration variations for ionic species and a constant permeate flux, aiming to provide insight in scaling potential. Alhseinat and Sheikholeslami [16] developed a model based on locally averaged CP for various feed water compositions, to evaluate scaling potential along a full-scale plant. While these models provide an estimate of axial gradients of solute concentration or degree of saturation (*DS*), no kinetic effects for actual precipitation are accounted for. The importance of precipitation rates in membrane systems has been illustrated by several researchers [17,18]. Only recently, efforts were made to develop numerical models coupling rates of nucleation and crystal growth with local solute concentration at the membrane [14,19]. Lyster et al. [14] developed a three-dimensional (3-d) numerical model for concentration polarization mapping at the membrane surface in a plate-and-frame flow cell, showing a correlation between crystal position (experimentally observed) and local degree of saturation (calculated with the model). In addition, the model reproduced experimental flux decline based on a simple mechanism of surface blockage by precipitate mapped according to visual observations. Lyster [20] further increased the model complexity, including crystal nucleation and growth in time. However, the rates of nucleation and crystal growth were evaluated based on the steady state degree of saturation distribution determined in the absence of any precipitate. Furthermore, only a single generic salt ($CaSO_4$) was assumed for all calculations. Karabelas et al. [19] and Kostoglou and Karabelas [21] proposed a mean field model for calcite precipitation in dead-end filtration, eliminating the complexity of the flow encountered in cross-flow filtration systems. Considering a simplified chemical system, their model accounts for bulk and surface nucleation and crystal growth based on the local salt concentration. However, Karabelas et al. [19] emphasized the importance of local hydrodynamics and mass transfer on the local degree of saturation of potentially scaling compounds.

There is a need for rigorous mechanistic modeling approaches that allow the detailed description of multiple factors governing scaling in a complex process like membrane filtration. In addition, the model should be applicable to a variety of feed water compositions. The objective of this work is to develop a micro-scale numerical model for studying mineral precipitation in RO/NF feed channels. A novel method is proposed, which combines physical and chemical processes in a numerical framework and aims at describing small-scale effects in relation to overall process performance.

2. Model description

The numerical model was developed to study fouling due to salt precipitation (mineral scaling) in the feed channel of a reverse osmosis system. The crystal nucleation and growth are coupled with the mass transport of solutes and fluid flow. Gypsum was chosen here as model precipitate, because it is a commonly occurring scale in many types of water [4,22]. Moreover, gypsum precipitation has been the object of many experimental studies and kinetic parameters for nucleation and growth are available. In addition, sodium chloride (NaCl) was chosen as additional solute, because it is one of the main contributors to total dissolved solids (TDS) in brackish water and seawater [1]. The numerical framework can be naturally extended to other scale forming salts (i.e., barium sulfate $BaSO_4$, calcium carbonate $CaCO_3$, silica SiO_2 or phosphates).

2.1. Model geometry

Due to the presence of feed spacer filaments in spiral wound modules the hydrodynamic conditions and solute distribution in the RO feed channel are considerably more complex [23–25] than it is assumed in simplified one-dimensional (1-d) models. However, given the complexity of the physical processes taken into account, the use of a fully 3-d geometry requires large computational resources and long simulation times, without providing much more insight at the qualitative level. Therefore, a two-dimensional (2-d) geometry is considered in this work, similar to the biofouling model presented in Radu et al. [24]. The simplest model geometry we used is representative for a plate and frame flow cell, containing two parallel flat sheet membranes that form the feed channel [10,26–28]. To better approximate real RO systems, more complex 2-d geometry including feed spacer filaments were also considered in this work. Feed channel and spacer geometrical characteristics (diameter of the filament, distance between consecutive filaments, orientation) are identical those used in other numerical studies [23,24] and listed here in Table 1.