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Dynamic operation of flat sheet desalination-membrane elements: A comprehensive model accounting for organic fouling

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ABSTRACT

Reliable simulation of membrane-module dynamic operation is essential in optimizing its detailed geometric characteristics and operation, as well as that of membrane plants, for various types of fluid treatment applications. This paper is part of systematic efforts toward development of such a comprehensive model, considering temporal variability caused by organic membrane fouling. To render the mathematical problem tractable, justified simplifications (retaining the physical parameter interdependencies) lead to a system of basic equations in two spatial planar coordinates, enabling to obtain a realistic temporal evolution of all process parameters. The flexible model structure allows integration of submodels, for phenomena occurring (and researched) at small spatial scales, which account for retentate spacer effects on friction losses and mass transfer, and constitutive expressions for fouling rates during desalination. The robust numerical algorithm developed to solve the system of differential and algebraic equations exhibits satisfactory convergence, appropriate for applications. The results presented herein demonstrate the versatility of the numerical code and its potential to analyze the interaction of mechanisms involved in fouling evolution, which is impossible by the much simpler one dimensional models. Directions for future developments are indicated.

1. Introduction

The very rapid expansion of membrane technology, in the past two decades, for various types of water treatment applications (e.g. desalination of brackish and sea water, effluent purification for reuse) has relied to a large extent on the use of flat-sheet spiral wound membrane (SWM) elements (Fritzmann et al., 2007; Greenlee et al., 2009). These SWM elements (well established in industry) facilitate the construction of rather flexible and *modular* desalination and water treatment plants, with production capacities that can vary at present in order of magnitude from 1 m^3/day to 10^6 m^3/day (e.g. Greenlee et al., 2009; Kurihara and Hanakawa 2013). The SWM modules are characterized by an ingenious design leading to high membrane packing density (in active membrane area per unit volume), which involves flat membrane sheets with thin spacers in-between (Karabelas, 2014) wrapped around a perforated central tube where the clean permeate is collected. The development of SWM modules to their presently marketable forms has been largely driven by the industrial needs, and facilitated by the accumulated technological experience over the years, with notable contributions from scientific research in the field of membrane materials (Elimelech and Phillip, 2011) as well as on membrane fouling and scaling and methods for their mitigation (Karabelas, 2014; Elimelech and Phillip, 2011). Moreover, it is well recognized that the complicated flow field in SWM modules and the spatially varying (even at steady state operation) process conditions are inadequately understood and modeled despite significant efforts especially during the past two decades (Karabelas et al., 2015). Recent relevant studies (Karabelas et al., 2014; Kostoglou and Karabelas 2013) and a state of the art review (Karabelas et al., 2015), regarding the effects of SWM module design parameters on its performance, show that significant progress has been made in developing a reliable steady-state simulator, and that a much needed for practical applications and research studies dynamic simulator (presently unavailable) requires a great deal of systematic development work. This study aims to contribute toward development of a comprehensive SWM dynamic simulator, by considering typical organic membrane fouling, which is a common cause for membrane plant temporal performance variability.

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The optimization of structural design, control and operation strategy of the membrane module requires the use of sufficiently detailed mathematical models in order to understand and quantify the interaction between the equipment design parameters and the process variables (Karabelas et al., 2015). A generalized mathematical modeling approach to membrane separation can be found in Marriott et al. (2001). However, the recent trend is to focus to specific details of each particular membrane process (Barello et al., 2015; Cao et al., 2016; Gurreri et al., 2016). Generally, the mathematical models can be of several degrees of complexity from simple integral (lumped parameter) to quite fundamental (first principles) approaches. However, the problem at hand is too complicated to allow a direct first principles approach; thus, a "divide and conquer" strategy is deemed necessary in order to handle efficiently several particular processes (sub-processes) occurring at different length and time scales. Specifically, the adopted approach is to derive constitutive expressions for the sub-processes based either on detailed subscale theoretical studies (wherever possible) or alternatively on experimental investigations for complex phenomena. Such an approach has been successfully followed in a previous publication (Kostoglou and Karabelas, 2013) for the development of a steady state SWM model, applicable to a clean membrane (i.e. no fouling occurring). The need to model the dynamic operation of SWM modules adds very significant complexity, i.e. the time varying module fouling must be accounted for. Four types of fouling are observed during SWM module operation: 1) scaling due to sparingly soluble salts (Hasson et al., 2001), 2) organic gel-layer formation (Schafer et al., 1998), 3) biofouling (Vrouwenvelder et al., 2009), 4) colloidal particle deposition (Yiantsios et al., 2005). The effect of the deposits is to increase the effective membrane resistance to permeation, to reduce the flow cross-sectional area in the retentate channels and to decrease the mobility of the solute, thus increasing concentration polarization. To systematically attack this problem, the present work is focused on the organic fouling which is the simplest to be modeled among the four fouling types. Therefore, the scope of this publication is to present the development of a dynamic model of SWM operation accounting for organic fouling, based on the previous steady state model (Kostoglou and Karabelas, 2013), and demonstrate its function as well as its capabilities; such a detailed dynamic model is unavailable at present. An ongoing assessment of the key system design and operating parameters on the SWM module dynamic performance (due to organic fouling) will be reported in a companion paper.

This paper is structured as follows: First, the model extensions with respect to the clean membrane case are discussed and the corresponding constitutive laws are suggested. Next, the dynamic model system of equations is presented and non-dimensionalized and the procedure for its solution is described. Finally, several characteristic model results are presented and discussed for two types of SWM-module operation, i.e. for steady state with a spatially non-uniform fouling layer and for dynamic module operation with a growing fouling layer.

2. Problem formulation

The dynamic model developed here is an extension of the steady state model presented in Kostoglou and Karabelas (2013), where the field variables are averaged in the transverse to the main flow direction, i.e. over the channel gap. The main features of the particular model include: (i) The capability to treat the two dimensionality of process parameters (throughout a membrane) induced by the finite pressure drop in the permeate channel, done in a detailed manner avoiding usual approximations (Schwinge et al., 2004; Avlonitis et al., 2007). (ii) The quasi-formal link to the equations describing in detail the transport process in the SWM module. (iii) The integration of sub-scale models and relevant expressions experimentally obtained in the authors laboratory. The model will be subsequently extended with the same degree of sophistication and in the same spirit of using appropriate subscale expressions based on detailed theoretical and experimental work. A first effort to simulate organic fouling evolution throughout a membrane sheet (Kostoglou and Karabelas, 2012) was restricted to the case of one-dimensional treatment of the retentate side and to the absence of solute to be separated from the feed. The results were encouraging, offering insights into the system dynamics and modeling issues, but the focus was not on model development leading to realistic simulation of SWM module operation.

The essential feature of the present model is the temporal variability of all process parameters caused by the growth of the organic fouling layer. Unlike the complexity of the other fouling modes, the mechanism of organic fouling appears to be rather straightforward. Indeed, the organic molecules are transferred to the membrane surface, aided by the normal permeation velocity, and adhere onto the membrane and further to the developing fouling layer. For major classes of foulants, it is realistic to consider *total* organic species rejection and no mass detachment (from the rather coherent fouling layer) by the shear stresses of the retentate cross-flow. Therefore, the local layer growth rate is taken proportional to the local permeate flux. Extensive experimental work performed in the authors laboratory (Sioutopoulos et al., 2010a,b) and elsewhere (e.g. Lee and Elimelech, 2006; Ye et al., 2005) shows that the above rather simple fouling mechanism can adequately describe reverse osmosis and nanofiltration membrane fouling by common organic matter, such as polysaccharides and their mixtures with humic acids. Further, there are several important issues, associated with the effect of a developing fouling layer on the SWM module performance, which should be examined (as follows) before proceeding with the derivation of the governing equations.

2.1. Extensions/Constitutive laws

The first issue concerns the *effect of the fouling layer on the pressure drop* in the retentate channel. The spacer filament diameter is denoted by D and it is by construction roughly equal to half of the retentate channel thickness. Assuming that the fouling layer has a uniform thickness h in the scale of the original *unit cell* (i.e. the elementary unit of the pattern formed by the crossing spacer filaments; Koutsou et al., 2007), a new unit cell must be considered in which the spacer-filaments exposed to flow will have cross sections of a circular segment (reduced by the part "immersed" in the fouling layer). However, the pressure drop relation for specified spacer type was determined by performing unit cell CFD simulations (in absence of fouling) and it was written in terms of a friction factor as f = f(Re) where Re is the Reynolds number based on D and on the local transversely averaged velocity (Koutsou et al., 2004; Koutsou et al., 2007; Ranade and Kumar, 2006). With a fouling layer, a new geometric parameter h/D should be added to the unit cell problem, and a modified constitutive relation of the form f = f(Re, h/D) is needed. In principle, such a relation can be determined by performing CFD simulations for several values of the parameters Re and h/D of the modified geometry. This type of simulations, involving a significant amount of work, will be performed in the future. At this stage an empirical closure of the constitutive relation will be pursued. For a clean membrane surface (h = 0), the relation between the retentate side pressure p and cross-flow velocity U is of the form (Kostoglou and Karabelas, 2009):

$$\frac{dp}{dx} = -\frac{f_1 U^{2-f_2} \rho^{1-f_2} \mu^{f_2}}{D^{1+f_2}} \tag{1}$$

where the dimensionless constants f_1 and f_2 depend on the type of the spacer (Koutsou et al., 2007). The constant f_2 takes values from 1