Journal of Membrane Science 515 (2016) 245–257

Contents lists available at ScienceDirect

Journal of Membrane Science

journal homepage: www.elsevier.com/locate/memsci

Active learning assisted strategy of constructing hybrid models in repetitive operations of membrane filtration processes: Using case of mixture of bentonite clay and sodium alginate

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ARTICLE INFO

Article history:
Received 27 September 2015
Received in revised form
28 May 2016
Accepted 31 May 2016
Available online 3 June 2016

Keywords:
Active modeling
Gaussian process regression model
Hybrid model
Membrane filtration processes
Transmembrane pressure

ABSTRACT

Reliable prediction of the transmembrane pressure (TMP) in membrane filtration systems often encounters different challenges in practice, including process nonlinearity, cycle-to-cycle change, and multiple operating conditions. In this work, an active learning TMP model with the hybrid structure is developed to predict the short-term fouling formation. The advantages of the physical and empirical models are integrated into this hybrid model. For construction of the empirical model, the Gaussian process regression model (GPRM) is adopted to approximate the complex fouling mechanism with fouling propensity in the short-term period. It can be a useful complement to the physical model with inaccuracy. Moreover, GPRM can simultaneously provide the prediction variance. Using this appealing property, the hybrid TMP model can be updated in an active and efficient manner without introducing additional unnecessary data samples. Consequently, accurate hybrid TMP models for the repetitive operations of membrane filtration processes are established. The superiority of the proposed hybrid TMP models is demonstrated through simulation and short-term experiments. The experimental results show the hybrid TMP models have better prediction performance (with R^2 values larger than 0.9) than the physical model (with R^2 about 0.5).

1. Introduction

During the last two decades, membrane technology has been increasingly applied to the treatment of different water sources, including wastewater and seawater. Membrane filtration is employed to separate particles, such as solid particles, colloids, macromolecules or molecules from a feed fluid [5,29]. Generally, the membrane will gradually lose its performance over a period of time, depending on the membrane type, materials in the feed, and process conditions. Membrane fouling is typically caused by inorganic and organic materials presented in water that adhere to the surface and pores of the membrane. It is an important but unavoidable problem associated with the application of membranes. It results in deterioration of the performance (e.g., reduced membrane flux) with a consequent increase in costs of energy and membrane replacement [1,24,35,48,5].

Control of fouling is of utmost importance. There are numerous research papers on fouling reduction. Cleaning of the fouled membranes has been widely studied in academia and industries [1,19,28,35]. Generally, mechanisms for membrane fouling are complex because they largely vary with hydrodynamic conditions, foulant-membrane and foulant-foulant interactions [24,48,5]. Chemical and physical cleaning methods have been utilized to eliminate fouling. There are still some problems associated with chemical cleaning, such as degrading some membranes and causing corrosion in the system [28]. Compared to chemical cleanings taken in a relatively low frequency, there are several physical methods, including hydraulic cleaning, pneumatic cleaning, and ultrasound cleaning for limiting membrane fouling during the operation. Backwashing is a typical physical cleaning method for pressure-driven membrane filtration processes [48]. And it can be used to remove most of the reversible fouling caused by pore blocking and to partially dislodge loosely attached sludge cake from the membrane surface [46]. During backwashing phases, the flow direction through the membrane is reversed so that the membrane pores can be flushed with permeate [19,46,5].

Abbreviations: GPRM, Gaussian process regression model; NN, neural networks; PLS, partial least squares; PVDF, polyvinylidene fluoride; TMP, transmembrane pressure

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http://dx.doi.org/10.1016/j.memsci.2016.05.057
0376-7388/

The behavior of flux decline needs to be investigated in order to prevent flux decrease. Additionally, accurate modeling of flux decline is crucial for further simulation, process design, control, optimization and scale up. Therefore, various flux decline models have been developed. Generally, from a modeling point of view, a process model can be constructed based on a first-principles model. The first-principles model can describe the fundamental phenomena of membrane fouling and performance. For example, the Darcy's law can describe the main phenomena of the transmembrane pressure (TMP) occurring in the filtration process. However, first-principles models are not capable of predicting the filtration flux precisely, because during filtration they require prior knowledge about the intrinsic nature of membranes, the behavior of particles to be separated, and the complex nature of forming the cake layer, which depends on hydrodynamic phenomena [15,42]. There are various complex phenomena effecting flux in a membrane filtration process and until now, none of the models are able to fully and satisfactorily describe the membrane filtration process in industrial processes [14,35,48].

Data-driven empirical models are alternative methods. Compared to first-principles models, data-driven empirical models can generally be developed quickly without requiring substantial understanding of the phenomenology. During the last two decades, data-driven modeling methods have been considered as useful alternatives for online prediction of flux and TMP in cross-flow microfiltration processes [11,12,15,16,18,2,3,8,10,23,25,30,34,40,42,43]. Current popular methods are neural networks (NN), including multilayer feed-forward NN [12,13,15,16,2,25,30,3,32,40,8], radial basis function NN [10,30], and several modified/improved NN methods [11,18,22,41]. The results show that NN is an effective nonlinear modeling tool in membrane filtration processes. Additionally, several statistical modeling approaches, such as partial least squares (PLS) and principal component analysis, have also been applied to membrane filtration processes with favorable effects [23,33,34,36,37,47].

Despite the nonlinear modeling ability of NN, the determination of the network topology for a complex modeling task is still not easy [20]. PLS and other multivariable statistical modeling are linear approaches; they are insufficient to capture the nonlinear relationship in the fouling mechanism. Furthermore, all of the previous empirical models (including NN and PLS) are deterministic, so the probabilistic information of its prediction is not provided. Accordingly, a large amount of data samples are required mainly because it is difficult to evaluate the prediction uncertainty of a model. To overcome these problems, a novel probabilistic method named Gaussian process regression model (GPRM) is first proposed in this work to model and predict the time evolution of TMP in the cross-flow membrane filtration. Compared with NN, the GPRM can automatically optimize its parameters with an iterative method [39]. As a result, it can be trained in an easy manner. Additionally, GPRM can simultaneously provide the probabilistic information of its prediction. Recently, GPRM has been applied to several chemical process modeling problems [17,26,27,31,9]. However, to our best knowledge, GPRM and its interesting probabilistic property have never been investigated to address membrane filtration processes.

Although many data-driven empirical models have been applied to the cross-flow microfiltration performance prediction, most of them are purely black-box approaches. The available knowledge of a process is not efficiently utilized. As aforementioned, first-principles models can generally describe the fundamental phenomena of membrane fouling. Data-driven empirical models, on the other hand, are suitable to predict complex behaviors in nonlinear processes [21]. Instinctively, both advantages of first-principles and data-driven empirical models should be integrated to enhance the prediction performance. Several applications of hybrid models to other chemical processes showed that they could predict the process states better than data-driven empirical models using solely on NN approaches [44,45]. In the previous membrane modeling studies, there were only a few hybrid (i.e., grey-box) models that can predict membrane fouling and performance [21,38]. Piron et al. [37] applied NN to estimate the parameters in a physically flux model. The results showed that the hybrid approach, as a means for complementing the description of a physical model, appears to be more accurate than the purely physical one. This can be considered as the serial structure of a grey-box model combined with NN [44,45]. For some complex membrane filtration processes, description of the entire process in the serial structure is not available. In this situation, an alternate parallel one can be adopted. In this study, to explore the potential of the combination of first-principles and empirical models, a hybrid GPRM-based prediction model with the parallel structure is developed to represent cake-layer formation and predict fouling propensity (i.e., short-term fouling formation). The traditional NN-based training methods often adopt all the training data. Unlike the traditional methods, the proposed method trains and updates the hybrid GPRM prediction model without introducing unnecessary data samples, so describing TMP accurately for the sequential operations of membrane filtration processes becomes relatively simple.

The remainder of this work is briefly structured as follows. The membrane filtration experimental system is described in Section 2. Section 3 describes and analyzes the physical TMP models for membrane filtration processes. Then, the proposed hybrid GPRM-based prediction models and the active updating strategy are developed. In Section 4, simulation results were first provided to show the advantages of the hybrid prediction models. Furthermore, the experiments described in Section 2 were conducted to evaluate the hybrid models. Finally, the conclusion is made in Section 5.

2. Materials and procedures

2.1. Colloidal suspensions

Ideal colloidal suspensions were prepared for flux tests using the mixture of bentonite clay (Kokusan Chemical Works, Ltd., Tokyo) and sodium alginate (Kokusan Chemical Works, Ltd., Tokyo) to generate a combination of particulate and macromolecular foulants. Bentonite clay of 25–33 μm in diameter was used as the model particulate solution. Sodium alginate was used as the model polysaccharide solution. 20 mg/L bentonite and 20 mg/L alginate solutions were used as the standard feed solution for the experiments in this study to simulate a combination of particulate and macromolecular foulants. To save experimental time and quickly collect the desired data, the operations within high suspended solid concentrations were made. This will easily show the deteriorated performance of the operations within a short duration.

2.2. Membrane materials

A polyvinylidene fluoride (PVDF) ultrafiltration membrane (Millipore) with a nominal pore size of 0.2 μm was used in this study. A sheet roll of the membrane was purchased, and membranes of the required size were cut for the experiments. All membranes were conditioned prior to being used by presoaking for four hours in ethanol. The length and the width of the membrane were 4 cm and 10 cm, respectively.

2.3. Experimental set-up and instrumentation, control and automation system

A laboratory-scale membrane filtration experimental system was designed and used to validate the proposed models in this