Hybrid model based expected improvement control for cyclical operation of membrane microfiltration processes
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HIGHLIGHTS
- The modeling method combines first principle models and the Gaussian process model.
- Handling the model mismatch can yield more accurate representation of the system.
- Expected improvement based control improves the economy of the process.
- Within-cycle control handles disturbances during the cycle.
- Experimental and simulation studies confirm applicability of the proposed method.

ABSTRACT
Membrane fouling can affect the performance of the membrane-based filtration. Fouling thus increases operational costs as a result of permeate flux decline and can be accompanied by increased energy load due to higher transmembrane pressure requirements needed as driving force. This work presents a modeling framework that combines first principle models with Gaussian process model and aims to account for model discrepancy due to the effect of fouling on the system from previous cycle of operation. Based on the expected improvement algorithm, a cycle-to-cycle in conjunction with a within-cycle optimization is proposed to handle the long duration of the operation to achieve the most economical operation in terms of energy load. Simulation studies as well as experimental studies have been carried out to show the applicability of the proposed method.

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1. Introduction
Membranes are widely used in drinking water applications to achieve improved removal of particulate matter, natural organic matter and salinity in water. The benefits of membrane based separation include low energy load, high selectivity and ease of operation (Farahbakhsh and Smith, 2006). Membrane-based technology also allows a smaller footprint for the treatment facilities compared to conventional treatment processes. As a result different types of membrane systems such as microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis are being increasingly applied to various industries such as food, pharmaceutical and chemical industries.

In membrane filtration the transmembrane pressure (TMP) difference forces the fluid and smaller particles through the membrane pores which then leave the system as permeate. The large particles are retained on the feed side. The filtration operation includes the dead-end-filtration and cross-flow-filtration. In dead-end-filtration, the feed flows parallel to the membrane pores. This operation is effective if the concentration of particles to be removed is low or the packing tendency of the filtered material does not produce a large pressure drop across the filter medium. In the cross-flow-filtration the feed flows perpendicular to the pores, rather than into it. The advantage of this is that the filter cake is substantially washed away during the filtration process, increasing the length of time that a filter unit can be operational. It can be operated continuously in contrast to the dead-end-filtration which is operated batch-wise.

Membrane fouling, which is the result of the accumulation of materials called foulants on the surface and/or in the pores of the membranes, can affect the performance of the membrane-based filtration. Many mechanisms contribute to membrane fouling, and their relative importance depends on the specific process. Six principal fouling mechanisms have been identified (Guo et al., 2012), including, (i) pore blocking: constriction of pore opening...
because of the deposition of particles around the pore entry, (ii) cake formation: formation of the layer because of the concentration of the repelled particles on the feed side, (iii) organic fouling: the dissolved organic matter attached to the membrane by adsorption, (iv) scaling: precipitation of inorganic substances on the membrane because of hydrolysis and oxidation during filtration, (v) biofouling: microorganisms adhering to the membrane and resulting in biofilm formation, and (vi) concentration polarization: back-diffusion away from the membrane induced by the concentration gradient of the retained substances. All of these phenomena reduce the process efficiency and they can be counteracted by membrane and module design, as well as by appropriate process control strategies (Busch et al., 2007). The typical fouling mechanisms for MF and UF are pore constriction, pore blocking, and cake formation. If the particles are smaller than the membrane pores, they can enter and stick to the pores. If the particles are about the same size as the membrane pores, the deposition of the particles onto the membrane surface may cause pore blocking. During the initial stages, membrane fouling is thought to be dominated by pore constriction and pore blocking (Chang and Fane, 2015). These decrease the performance and potentially damage the membrane. Fouling thus increases operational costs as a result of permeate flux decline and can be accompanied by increased energy load due to higher TMP requirements needed as driving force. The reversible fouling can be eliminated at least partially by aeration and backwashing (Yigit et al., 2009). In the backwashing phase, the flow direction through the membrane is reversed, such that the membrane pores are flushed with permeate. However, internal clogging of pores by the adsorption of colloidal and dissolved materials is more problematic, and can hardly be eliminated by vigorous chemical cleaning. The backwashing increases the costs of the operation. In addition, frequent chemical cleaning of fouled membranes leads to rapid deterioration of membrane performance, shortened service life, and increased costs. The efficient use of fouling controlling strategies can reduce the energy demand and other associated operational costs, and improve the sustainability of membrane based operation. This can be accomplished by optimizing the operation of membrane filtration processes through process control.

In industrial practice the filtration systems are usually controlled to meet the desired net flux. However the high complexity of the filtration process poses a challenge in control of the process. It is characterized by the periodic change between filtration and backwashing, by the drift of membrane permeability due to membrane fouling, and by a high-number of disturbances, including variations of temperature or solid concentration. Furthermore, in most cases, only the overall TMP across an entire membrane module is measured and thus that little information is available to describe the process. Development of models gives insight into the effects of control on the process and Smith et al. (2006) presented an online approach in which backwashing is initiated when the TMP has increased by a certain amount, which is advantageous as compared to backwashing at a fixed frequency. Blankert et al. (2006) developed a filtration model and determined the optimal profile of the filtration flux and TMP during one filtration phase using offline dynamic optimization. Busch et al. (2007) presented run-to-run control of membrane filtration processes. In their work the filtration process was divided into cycles and the model was updated using plant measurements of previous cycle to find the optimum manipulated variables for the cycle. Nevertheless, the occurrence of a mismatch between the predicted energy load – using parameters of the previous cycle – and actual current cycle energy load was not taken into account. This mismatch was the result of the model parameters differing with each cycle due to fouling and has to be taken into account to obtain the best performance of the filtration process. Robles et al. (2013, 2014) proposed a model based control and used online measurement to monitor the filtration through measuring the fouling rate online but sampling and analytical assay are required.

The methods to model the TMP can generally be classified as data driven or phenomenological/first-principled. First principle models (or physical models) use prior knowledge of the system to derive the mathematical representation that can describe the fundamental phenomena of the filtration process. For example, the Darcy’s law can describe the main phenomena of the transmembrane pressure occurring in the filtration process. However, until now, none of the models are able to fully and satisfactorily describe the membrane filtration process in industrial processes (Ferrero et al., 2012; Padaki et al., 2015; Zhang et al., 2015). On the other hand, data-driven modeling methods have been considered as useful alternatives for online prediction of flux and transmembrane pressure difference (TMP) in cross-flow microfiltration processes. Data driven models can generally be developed quickly without requiring substantial understanding of the phenomenology. Currently, neural networks (NN) are commonly used in membrane filtration modeling (Chen and Kim, 2006; Cheng et al., 2008; Ghandehari et al., 2011; Kaneko and Funatsu, 2013; Liu et al., 2009; Mirbagheri et al., 2015; Oishi et al., 2015). In addition, statistical modeling approach such as partial least squares (PLS) has also applied to membrane filtration processes (Kaneko and Funatsu, 2013; Oishi et al., 2015; Peiris et al., 2012). PLS modeling approaches are linear approaches and are unable to capture the nonlinear information in the fouling mechanism. NN can be used for nonlinear modeling but the determination of the network topology for a complex modeling task is still not easy (Huang et al., 2015). Furthermore, the data-driven 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.

The combination of both the first-principle and the data-driven empirical models in the hybrid model can thus be useful for control of membrane filtration. The hybrid model structure combines both advantages of first-principles and data-driven to enhance the prediction performance. First-principles models can generally describe the fundamental phenomena of membrane fouling. Data-driven models, on the other hand, are suitable to predict complex behaviors in nonlinear processes (Hwang et al., 2009). In membrane filtration, a number of works on using hybrid models to predict membrane fouling and performance (Hwang et al., 2009; Piron et al., 1997) have been reported. The results showed that the hybrid approach, as a means for complementing the description of a physical model, to be more accurate than purely physical one.

Optimization can then be performed based on the model to select subsequent search points. In an optimization context, this model can be viewed as a response surface. This method is potentially efficient if data collection is expensive relative to the costs of building and searching a response surface. In the response surface methodology a response surface is conducted and surface is searched for likely candidate points, evaluated according to some criterion. The expected improvement (EI) is a type of response surface methodology and it is based on the Gaussian process regression model (GPRM). Conventional method is deterministic but EI is probabilistic which takes into account the model uncertainty. GPRM is a probabilistic tool for nonlinear regression. GPRM can simultaneously provide the probabilistic information for its prediction (Rasmussen and Williams, 2006). The variance of the prediction can be interpreted as a confidence level of the model. Additionally, the number of GPRM hyper-parameters that need to be optimized is small compared to parametric approaches, such as NN. It has been increasingly considered as an alternative approach to NN (Neal, 1996) and it has been increasingly applied
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