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Time-Optimal Control and Parameter Estimation of Diafiltration Processes in the Presence of Membrane Fouling

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Abstract: This paper deals with the time-optimal operation and parameter estimation problem of a general diafiltration process in the presence of fouling. Fouling stands for one of the dominant problems in the membrane separation processes. The dynamic behavior of the fouled membrane is described by a general fouling model taken from literature. An Extended Kalman filter is proposed for the recursive estimation of unknown parameters in the fouling model. A model-based optimal nonlinear controller, whose control law is obtained explicitly via Pontryagin's minimum principle, is coupled with the parameter estimation and subsequently applied in a simulation case study to show benefits of the proposed approach.

Keywords: Kalman filter, batch diafiltration, optimal control, membrane fouling, parameter estimation

1. INTRODUCTION

Membrane processes employ perm-selective membranes to separate solutes in a solution based on differences in molecular size so that the high molecular weight components are retained on the feed side of the membrane and the low molecular weight components are able to pass through it. These processes have found a wide range of application in the pharmaceutical, food, and biotechnological industries (Cheryan, 1998).

A diafiltration is a membrane process that uses a solute-free solvent (diluant) to control the membrane process via influencing the concentrations of solutes. Several authors (Foley, 1999; Takači et al., 2009) showed that different strategies of diluant addition can result in different operational savings where time-optimal operation or minimal consumption of diluant can be achieved.

Ng et al. (1976); Takači et al. (2009); Paulen et al. (2012) optimized the final processing time and/or the consumption of the diluant. This includes the optimization of the switching times between the predefined operational modes, such as concentration, constant-volume diafiltration, application of sophisticated numerical and analytical approaches. Our recent work (Paulen et al., 2015) showed that the two major optimization problems can be solved as a single optimization problem formulated in a multi-objective fashion where a use of Pontryagin's minimum principle allows to obtain analytical solutions for many common process setups.

Fouling behavior is one of main issues in membrane separation processes. It decreases effective membrane area due to the blockage of pores and results in a substantial increase of operational costs. The pioneering work of Hermia (1982) presented a unified fouling model describing this behavior. Recently, Charfi et al. (2012) showed that numerical optimization techniques can be employed to predict types of the fouling mechanism using experimental data of the permeate flow.

In our previous work of Jelemenský et al. (2015) we derived a fully analytical procedure for the time-optimal operation in the presence of the membrane fouling. However, optimal model-based control of membrane processes requires a knowledge of process model and its parameters where the use of inaccurate values of the parameters could lead to significantly suboptimal performance. Estimation of unknown parameters can be done using various methods. Common practice is to employ a least-squares method and to estimate multiple fouling models in parallel off-line (Charfi et al., 2012). More advanced methods include Kalman filtering or moving horizon estimation strategies (Alessandri et al., 2005).

In this paper we study the combined time-optimal operation of a batch diafiltration process and the estimation of fouling models and parameters using Extended Kalman Filter (EKF). The proposed scheme is attractive as it applies inherently robust nonlinear optimal feedback control with on-line estimation of process parameters. We will show that the estimation of the fouling behavior results in

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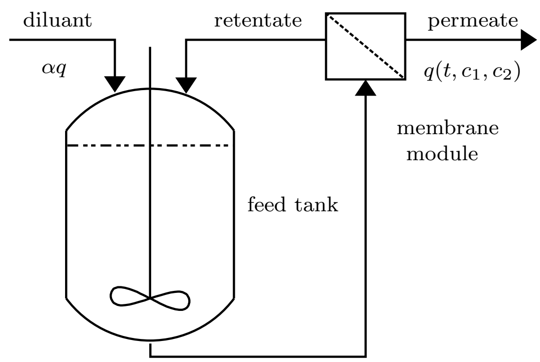

Fig. 1. Schematic representation of a generalized diafiltration process.

optimal control performance even if the fouling parameters are initially not known.

The paper is organized as follows. Section 2 describes the process and its model including a model of fouling behavior. Section 3 presents the formulation of the optimization problem and its analytical solution. An overview of EKF and its application to the studied problem is described in Section 4. The proposed approach is applied in a simulation study in Section 5. Section 6 concludes the paper.

2. PROCESS DESCRIPTION AND MODELING

In this paper we study a generalized batch diafiltration process represented in Fig. 1. We consider that the process runs under constant pressure and temperature. The diafiltration process involves a feed tank, where the solution that consist of two solutes is introduced, and a membrane. The feed is brought to the membrane and the stream rejected by the membrane (retentate) is taken back into the feed tank. The stream which leaves the system is called permeate and its flow-rate is defined as $q = AJ$, where A is the membrane area and J is the permeate flux subject to unit membrane area. The permeate flux can be a function of solutes concentrations and time.

The control of the diafiltration process can be achieved by adding a solute-free solvent (diluant) into the feed tank. The control variable α expresses the ratio between the inflow of diluant and the outflow of the permeate q. In the industry, there are traditionally used control modes which differ in the rate of diluant addition. A mode with $\alpha = 0$, during which no diluant is added into the feed tank, is called concentration (C) mode. The second traditional mode is constant-volume diafiltration (CVD) where $\alpha = 1$ and during this mode the inflow of dilaunt is kept the same as the permeate outflow. Dilution (D) mode is characterized by $\alpha = \infty$ where a certain amount of diluant is added into the feed tank. A typical industrial control strategy consists of a sequence of the aforementioned control modes (e.g. C-CVD).

The mass balance for the individual solutes can be written as (Kovács et al., 2009)

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = \frac{c_i q}{V}(R_i - \alpha), \quad c_i(0) = c_{i,0}, \quad i = 1, 2, \tag{1}$$

where V stands for the volume of the feed at time t and subscript i denotes the macro-solute and micro-solute, respectively. R_i is the so-called rejection coefficient. The rejection coefficient is a dimensionless number between 0 and 1 that measures the ability of the membrane to reject a particular solute.

The total mass balance can be written as

$$\frac{\mathrm{d}V}{\mathrm{d}t} = u - q = (\alpha - 1)AJ, \quad V(0) = V_0, \tag{2}$$

with V_0 being the initial volume of the processed solution.

Moreover, the rejection coefficient R_i can be a constant or a function of both concentrations. In the remainder of the paper we will consider that the rejection coefficients are constant ($R_1 = 1$ and $R_2 = 0$). This means that the membrane is perfectly impermeable for the macro-solute and that the micro-solute can freely pass through the membrane pores. Since the rejection for the macro-solute is equal to one, the total mass in the system will not change and stays constant ($c_1(t)V(t) = c_{1,0}V_0$). This allows us to eliminate the differential equation for the volume (2). Then, the equivalent model has the following form

$$\frac{\mathrm{d}c_1}{\mathrm{d}t} = \frac{c_1^2 AJ}{c_{1,0}V_0}(1 - \alpha), \qquad c_1(0) = c_{1,0}, \tag{3}$$

$$\frac{\mathrm{d}c_2}{\mathrm{d}t} = -\frac{c_1 c_2 AJ}{c_{1,0}V_0}\alpha, \qquad c_2(0) = c_{2,0}. \tag{4}$$

2.1 Membrane Fouling

The membrane fouling depends on several properties such as feed concentration and viscosity, membrane material, temperature, and pressure. Fouling causes the decrease of the effective membrane area due to the deposit of the solutes in/on the membrane. A unified model of the fouling behavior was derived by Hermia (1982) in terms of the total permeate flux and time and reads as

$$\frac{\mathrm{d}^2 t}{\mathrm{d}V_\mathrm{p}^2} = K\left(\frac{\mathrm{d}t}{\mathrm{d}V_\mathrm{p}}\right)^n, \tag{5}$$

where V_p represents the permeate volume, t is time, and K is the fouling rate constant. The parameter n determines the type of the fouling mechanism where four classical fouling models can be recognized: cake ($n = 0$), intermediate ($n = 1$), standard (internal) ($n = 3/2$), and complete ($n = 2$) fouling model.

Equation (5) can be rewritten as as (Vela et al., 2008)

$$\frac{\mathrm{d}J}{\mathrm{d}t} = -KA^{2-n}J^{3-n}. \tag{6}$$

and it can be solved for a particular choice of n to yield

$$n = 0: \qquad \frac{1}{J^2} = \frac{1}{J_0^2} + K_g t, \tag{7a}$$

$$n = 1: \qquad \frac{1}{J} = \frac{1}{J_0} + K_i t, \tag{7b}$$

$$n = \frac{3}{2}: \qquad \frac{1}{\sqrt{J}} = \frac{1}{\sqrt{J_0}} + K_s t, \tag{7c}$$

$$n = 2: \qquad \ln J = \ln J_0 - K_c t, \tag{7d}$$

where J_0 is the initial flux and K_g, K_i, K_s, K_c are respective fouling constants for the different values of n.

Fig. 2 shows a graphical representation of these fouling mechanisms. The distinguishing feature of the models is present by the way the molecules deposit in/on the