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Economically optimal batch diafiltration via analytical multi-objective optimal control

R. Paulen[a,b,*], M. Jelemenský[a], Z. Kovács[c], M. Fikar[a]

[a] Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinskeho 9, Bratislava, Slovakia
[b] Department of Chemical and Biochemical Engineering, Technische Universität Dortmund, Emil-Figge-Strasse 70, Dortmund 44221, Germany
[c] Department of Food Engineering, Corvinus University of Budapest, Ménesi 44, 1118 Budapest, Hungary

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ABSTRACT

This paper studies the problem of economically oriented optimal operation of batch membrane diafiltration processes that are designed to concentrate the valuable components of the solution and to purge the impurities from it. We consider a complex economical objective that accounts for the total operational costs comprising a cost of consumed diluant, costs related to duration of processing, and a cost of product loss. The optimization problem is formulated as a multi-objective optimal control problem in order to investigate the impact of operational cost factors on optimal operation policy. This is achieved thanks to the use of the analytical approach that exploits Pontryagin's minimum principle. We show that the economically optimal control strategy is to carry out an operation involving saturated (bang-bang or constraint-tracking) control modes and a singular arc. For the most common cases of diafiltration problems, it turns out that the switching of the consecutive control modes can be realized in the state feedback fashion, i.e. the entire optimal operation is defined analytically in the space of process states. We demonstrate the applicability of the presented approach and we illustrate achievable benefits, over traditional control methods for the batch diafiltration processes, on two case studies taken from the literature.

1. Introduction

Diafiltration (DF) is known as an effective membrane process for separation of two or more solutes from a solution. Currently, it is well-established in chemical, biochemical, food and pharmaceutical industry [1]. Its aim is the increase of concentration of a desired product together with the simultaneous decrease of concentration (washing-out) of impurities in a solution. This goal is achieved by employing pressure-assisted separation via a perm-selective membrane. The applications of DF encompass fractionation and purification of proteins [2,3], albumin production from human blood plasma for medical use [4], separation of protease from tuna spleen extract [5], production of recombinant DNA derived human protein pharmaceuticals [6] and antibody preparation [7]. In enzyme biotechnology, it is used to concentrate enzymes and to remove peptides, oligosaccharides, salts, and other metabolic impurities [8,9]. Some of the other important applications include, for example, virus harvest and purification [10,11], desalination of various pigments [12] and gelatin [13], purification of nanoparticles [14,15], treatment of bleach plant effluents [16], and fruit juice clarification [17].

Pressure-driven membrane filtration is considered to be a mature technology, however broad optimization and innovation potential exists. Reducing operational costs is a key to fully exploit this technology and to make it competitive and sustainable for the future. Improvement potential can be discovered via analysis of the operational degrees of freedom that are available to steer the operation towards the optimal resource allocation and energy utilization. In principle, there are two control loops in operation of the batch DF processes that assign available degrees of freedom. The low-level one takes place in order to ensure the maintenance of desired separation performance of the membrane by adjusting the hydrodynamic conditions in the system. Strategies such as constant flux, constant transmembrane pressure, or constant membrane wall concentration [6] are of a usual choice in the industrial practice. The high-level control loop decides about utilization of so-called wash-out (diafiltration) water, i.e. a solute-free solvent or diluant. By choosing the right diluant utilization policy, we may

* Corresponding author at: Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinskeho 9, Bratislava, Slovakia.
Tel.: +421 259 325 730; fax: +421 259 325 340.
E-mail address: radoslav.paulen@stuba.sk (R. Paulen).

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dynamically influence the concentrations of species in the system and, thus, further enhance the performance of the membrane separation, thus the economics of the process. Our present study deals with the optimization and further analysis of economic operation of batch DF subject to the rate of utilization of diluant throughout the course of the batch run.

State-of-the-art schemes of diluant utilization, proposed in the literature [4,18], consider various combinations of three operational modes: concentration mode (C), constant volume diafiltration (CVD) mode, and variable volume diafiltration (VVD) mode. Resulting operational policies are simple from a viewpoint of their implementation, however, generally suboptimal due to arbitrary pre-selection of the nature, order, and duration of the subsequent control modes [19].

The field of membrane engineering and membrane process control has generally received an increased attention of the researchers over the past years [20–22] where various advanced optimization and process control techniques were used in order to enhance the economics of running the membrane processes. Up to now, many attempts appeared in the literature to treat the problem of enhancement of economic optimality of DF processes. Developed approaches either optimize switching times between arbitrarily predefined operational modes [23,24,17] or they find approximations to optimal control numerically [25,26]. The present study builds upon our previous work [27] where optimal control was derived for minimum time and minimum diluant operations analytically using Pontryagin's minimum principle (PMP) approach. Here we generalize these findings by treating a complex multi-objective minimization of operational costs that involves terms related to processing time, to amount of consumed diluant, and to the loss of product. These terms are included in the objective while being regarded as proportional to the respective unit prices and, thus, a relevant metric is established for process operational expenses. Our aim is to solve the problem with undetermined weighting parameters in order to characterize the optimal operation for arbitrary unit prices. Such treatment allows for quick adaptation of the optimal operation to the varying economical aspects of the problem and market situations.

The studied problem of optimal operation of DF process is a problem of multi-objective optimal control. In recent years, several numerical approaches have been developed to treat this kind of problems. These approaches rely on efficient numerical solution of underlying optimal control problem and parametrization of the Pareto fronts [28–31]. Despite the substantial progress in numerical approaches to multi-objective optimal control problems, the application of such approaches might incur additional costs for computing hardware as well as hardware costs linked with implementation of the numerical solution. We focus, in this study, on analytical form of solving the multi-objective optimal control problem. Such approach provides an insight and understanding of the optimal operation while makes the implementation of the optimizing control policy realizable without any modifications to process control hardware.

We apply PMP in order to solve the arising optimal control problem analytically. More concretely, we derive the necessary conditions for optimality given by PMP and we identify resulting optimizing control policy with generalized weighting factors of the different objectives. It turns out that for the most common cases of DF process, relevant to practice, optimality conditions define the operation completely, i.e. the control structure (sequence of solution arcs) is identified together with the corresponding switching conditions as a function of importance of the different objectives expressed via weighting coefficients of the multiple objectives. In turn, this solution approach gives us an advantage to further analyze the effect of different operational aspects present in the objective function in the light of the analytical solution at hand.

This paper builds upon our preliminary results [32,33] and extends the derivation of the optimal operation of DF processes to cover a wider set of problems found in the literature and practice. It is organized as follows. In Section 2, we introduce the studied problem of economically optimal operation of generalized batch DF process. Section 3 gives the derivation and interpretation of optimality conditions using PMP. These are accompanied with the resulting optimal operation schemes generalized for different common process setups. Finally, we apply the method developed here to find an economically optimal diluant utilization strategy for the selected case studies of varying complexity relevant to industrial practice and we discuss the key benefits of presented approach and the resulting operation policies.

2. Problem statement

In this section, we give a description of a batch DF plant, we state the generalized model of the considered process and we define the goals that are to be reached by means of optimal control.

2.1. Process description

Fig. 1 shows a schematic diagram of a batch DF plant layout that is designed to reduce the processing volume, thus to achieve a certain concentration of valuable dissolved species, and to eliminate the impurities from the product solution. The applied membrane is selected to retain the product (hereafter referred to as macro-solute) while allowing undesirable impurities (hereafter, micro-solute) to pass through the membrane. In the operation, the solution is passed from the feed tank to the membrane module where permeate stream, of flowrate $q(t)$, leaves the system and the retentate stream is recirculated to the feed tank. During this process, fresh solute-free diluant stream (e.g. wash-water), of flowrate $u(t)$, can be added into the feed tank to replace solvent losses.

Achievement of good separation properties of the setup in Fig. 1 is predetermined by employing a well-suited (low-level) control of this process such as constant flux, constant pressure, or constant wall concentration control [34]. Selection of one of these control methods is in most cases done beforehand, at the process design phase, according to the filtered solution properties (such as density and viscosity) and overall expected system behavior. In contrast, dynamical response to the changes in the membrane performance throughout the process run can be then achieved by selection of right diluant utilization strategy. The scheme of diluant utilization is best described in terms of dimensionless variable α, as noted in Fig. 1, that is defined as the ratio of diluant inflow (u) to permeate outflow (q).

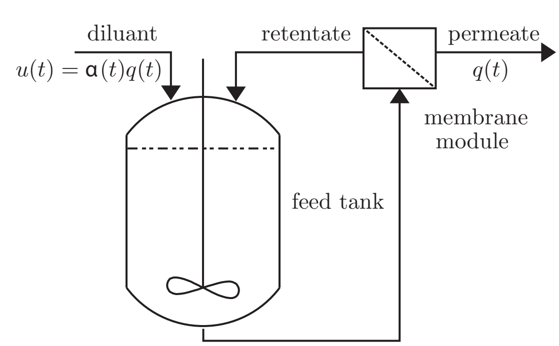

Fig. 1. Schematic representation of a batch diafiltration process.