Dynamic Optimization of Batch Membrane Filtration Process

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Abstract

We present a comprehensive mathematical model that can be used for simulation, optimization, and control of batch diafiltration processes. It unifies the existing models for classical diafiltration concepts. The model is used for determination of optimal operation of a specific separation design problem. Methods of dynamic optimization are employed to obtain optimal solutions. We show that conventional diafiltration techniques can but need not be optimal. The presented methodology is particularly applicable for decision makers to evaluate the optimal water utilization strategy for the given separation design problem.

Problem Statement

Membrane diafiltration is a widely-used separation technique that has found many applications in the food and beverage, chemical, biotechnological, and pharmaceutical industries. In this case study, we treat a problem of albumin-ethanol solution separation.

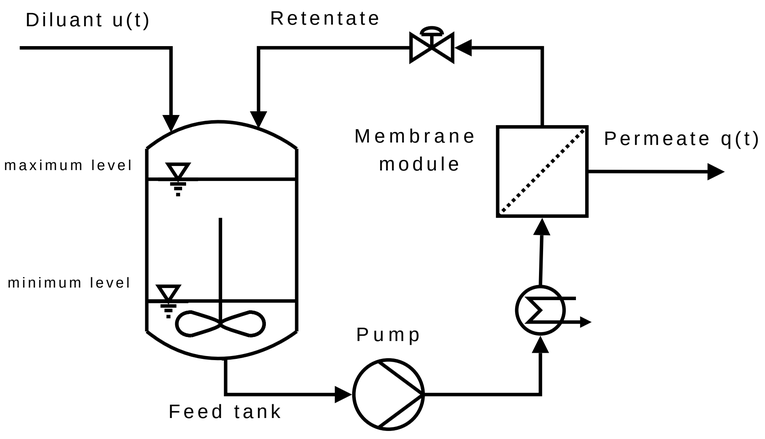

Figure 1: Batch membrane filtration system.

Process Model

The process dynamics can be described by the following first-order ordinary differential equations (ODE) with their corresponding initial conditions

$$\dot{V} = u - q(c_1, c_2), \qquad V(t_0) = V_0 \tag{1}$$
$$\dot{c}_1 = \frac{c_1}{V}\left[q(c_1, c_2)\mathcal{R}_1(c_1, c_2) - u\right], \qquad c_1(t_0) = c_{1,0} \tag{2}$$
$$\dot{c}_2 = \frac{c_2}{V}\left[q(c_1, c_2)\mathcal{R}_2(c_1, c_2) - u\right], \qquad c_2(t_0) = c_{2,0} \tag{3}$$

where V represents feed tank solution volume, u is fresh solute-free diluant volumetric flowrate, and q stands for permeate volumetric flow rate. $\mathcal{R}_1$ and $\mathcal{R}_2$ denote the rejection of macro-solute and micro-solute, respectively. In this specific application, however, the rejection of the macro-solute (i.e. albumin) is found to be unity, while the rejection of the micro-solute (i.e. ethanol) to be zero.

Control of diafiltration processes is traditionally operated using a dimensionless variable $\alpha(t)$ which is defined as a fraction between inflow and outflow

$$\alpha(t) = \frac{u(t)}{q(t)} \tag{4}$$

Introducing $\alpha(t)$ into Eq. (1)–(3) yields

$$\dot{V} = (\alpha - 1)q, \qquad V(t_0) = V_0 \tag{5}$$
$$\dot{c}_1 = \frac{c_1}{V}(1 - \alpha)q, \qquad c_1(t_0) = c_{1,0} \tag{6}$$
$$\dot{c}_2 = -\frac{c_2}{V}\alpha q, \qquad c_2(t_0) = c_{2,0} \tag{7}$$

The experimental investigation available in literature has shown that both albumin concentration c_1 and ethanol concentration c_2 considerably affects the permeate flow q.

$$q(c_1, c_2) = \frac{1}{b_1 + b_2 c_1 + b_3 c_2 + b_4 c_1 c_2 + b_5 c_1^2 + b_6 c_2^2} \tag{8}$$

Process Optimization

Fig. 2 shows traditionally used diafiltration schemes and it illustrates the new proposed one as well.

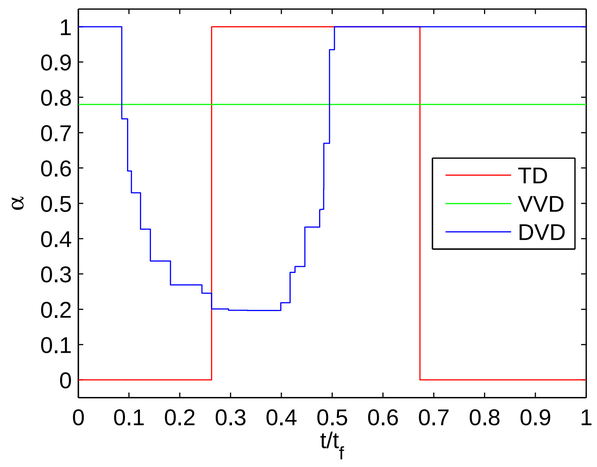

Figure 2: Diafiltration schemes – traditional diafiltration (TD), variable volume diafiltration (VVD), dynamic volume diafiltration (DVD).

Minimum Time Problem

The objective of this optimization task is to find the time dependent function $\alpha(t)$ which uses minimum time to drive the process from initial state to a prescribed terminal state.

$$J_1 = \min_{\alpha(t)} t_f \tag{9a}$$

s.t.

$$\dot{V} = (\alpha - 1)q, \qquad V(t_0) = V_0, \quad V(t_f) = V_0\frac{c_{1,0}}{c_{1,f}} \tag{9b}$$
$$\dot{c}_1 = \frac{c_1}{V}(1 - \alpha)q, \quad c_1(t_0) = c_{1,0}, \quad c_1(t_f) = c_{1,f} \tag{9c}$$
$$\dot{c}_2 = -\frac{c_2}{V}\alpha q, \qquad c_2(t_0) = c_{2,0}, \quad c_2(t_f) = c_{2,f} \tag{9d}$$

Minimum Diluant Problem

The second problem addresses minimization of total amount of diluant $u(t) = \alpha(t)q(t)$ used to drive the process from initial state to a prescribed terminal state assuming that the final time t_f is a free variable. Mathematical formulation (9) remains unchanged in this case except for the cost function

$$J_2 = \min_{\alpha(t)} \int_{t_0}^{t_f} \alpha(t)q(t)\mathrm{d}t \tag{10}$$

Results

We investigated several cases of prescribed initial process state and desired terminal state. Here, we document one of these for which the conditions were

$$c_{1,0} = 15\,\mathrm{kg\,m^{-3}} \quad \Rightarrow \quad c_{1,f} = 80\,\mathrm{kg\,m^{-3}}$$
$$c_{2,0} = 146.3\,\mathrm{kg\,m^{-3}} \quad \Rightarrow \quad c_{2,f} = 0.1\,\mathrm{kg\,m^{-3}}$$

Results show that process is speeded up about 10-15% by using DVD scheme in comparison with conventional techniques. Moreover, using of DVD scheme may save up to 69% of diluant.

Minimum Time Problem

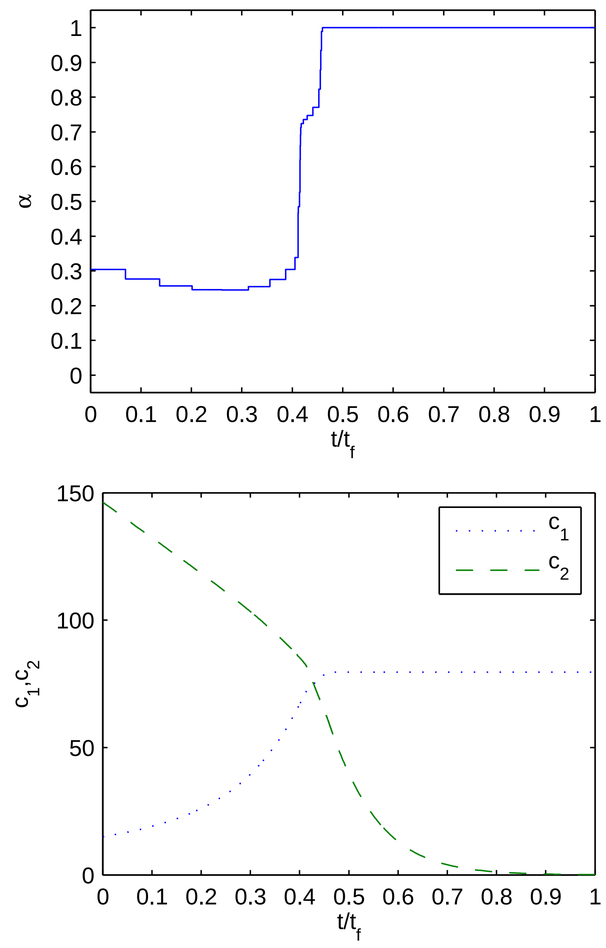

Figure 3: Graphical results for minimum time problem. ($J_1^* = 2.29\,\mathrm{h}$, $J_2 = 0.103\,\mathrm{m^3}$)

Minimum Diluant Problem

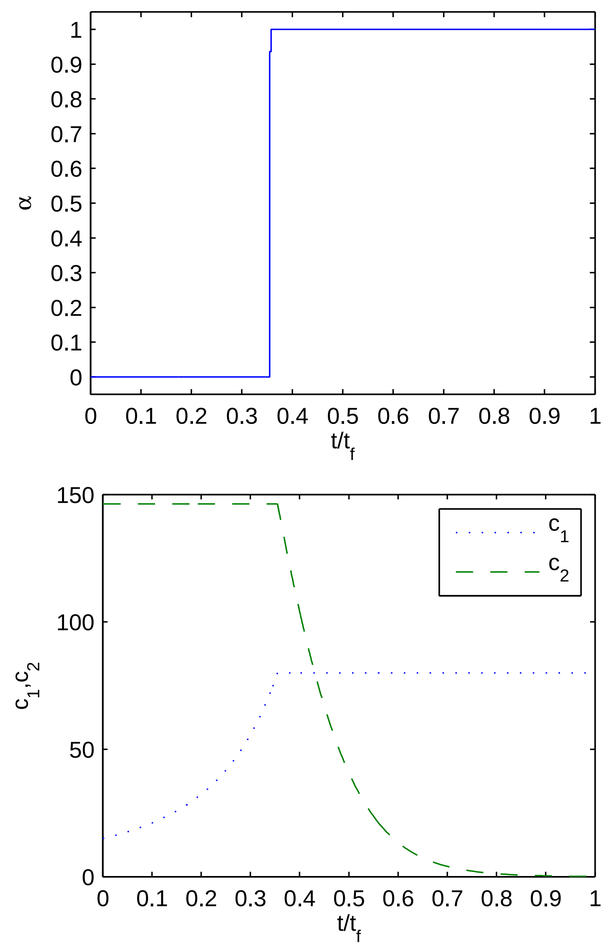

Figure 4: Graphical results for minimum diluant problem. ($J_1 = 2.31\,\mathrm{h}$, $J_2^* = 0.091\,\mathrm{m^3}$)

Conclusions

We presented a comprehensive mathematical model that can be used for simulation, optimization, and control of batch diafiltration processes. Methods of dynamic optimization were employed to obtain optimal solutions to different optimization problems. We have demonstrated the power of the proposed optimization method on two selected problems: minimum time and minimum diluant consumption problem, and investigated whether conventionally used diafiltration techniques can be considered as optimal. We found that two-step TD process, involving a pre-concentration and a constant-volume dilution mode step, is optimal in case of minimization of overall diluant consumption. However, obtained optimal trajectories can differ from the traditionally used operation in case of time minimization.

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