A unified modeling approach for the optimization of water usage in batch diafiltration processes

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Outline

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1. Motive of the Study
2. Diafiltration System Design
   - Operational Principle and Process Strategies
   - Mathematical frame for simulation
   - Mechanism-driven models
   - Data-driven models
3. Process optimization
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   - Optimal control profile
4. Summary

Outline

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Motive of the Study

Applications:

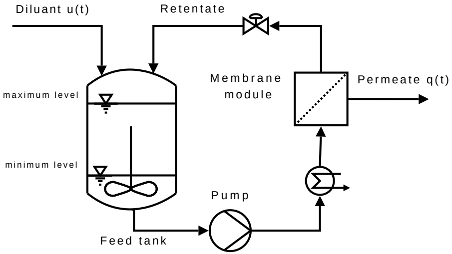
- NF separation of amino acid derivates from inorganic salts (industrial project - IVT Austria)
- MF separation of a ternary dispersed system containing an organic solvent, water and fine particles (industrial project - IVT Austria)
- UF separation of proteins from animal blood plasma (industrial project - IVT Austria)
- UF separation of enzymes from fermentation broth (industrial project - IVT Austria)
- Demineralization of whey with NF (research project - Corvinus Hungary/ IBPT Germany)
- Virus purification (research project - IBPT Germany)
- Concentration and purification of albumin by UF from albumin/ethanol/water system (research project - STU Slovakia/ IBPT Germany)
- UF separation under gel polarization conditions (research project - DCU Ireland/ STU Slovakia/ IBPT Germany)

Operational Principle

System: Aquoeus solution of micro- and macrosolutes.

Requirement: Low membrane rejection for micro- and high for macrosolutes.

Separation objective: Micro-component removal and macrosolute concentration.



Operational modes:

1. Concentration mode ($\alpha = \frac{u(t)}{q(t)}$=0)
2. Constant-volume dilution mode (α=1)
3. Variable-volume dilution mode (α=const $\in [0,1]$)

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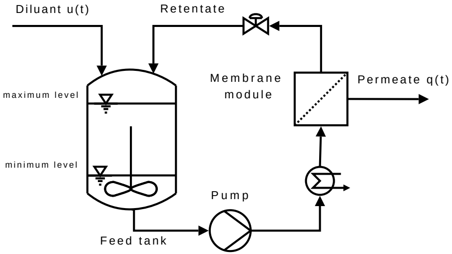

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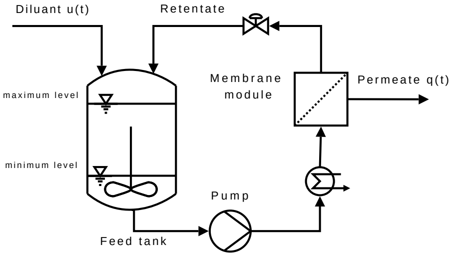

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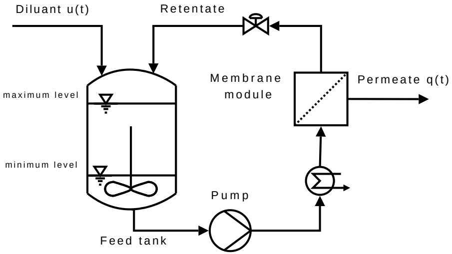

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Diafiltration concepts

Traditional Diafiltration (TD):

1. pre-concentration – 2. constant-volume dilution – 3. post-concentration

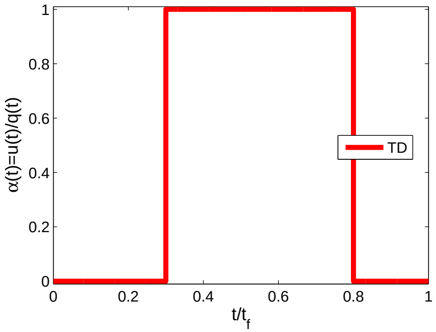

Figure: Control strategy: $\alpha = \{0, 1, 0\}$

Diafiltration concepts

Variable-volume diafiltration (VVD):

(1. pre-concentration) – 2. variable-volume dilution

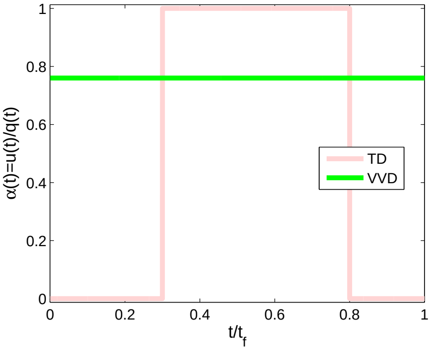

Figure: Control strategy: $\alpha = \{\alpha_k\}$ or $\alpha = \{0, \alpha_k\}$ where $0<\alpha_k<1$

Diafiltration Concepts

Dynamic-volume diafiltration (DVD):

optimal time-dependent profile of the diluant flow for the entire process

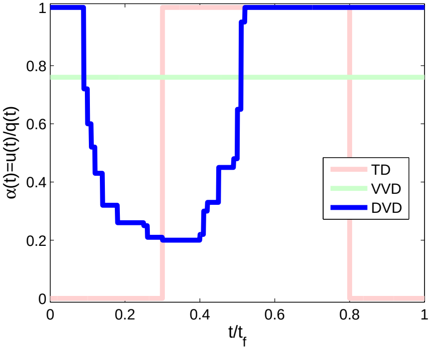

Figure: Control strategy: N x piece-wise constant $\alpha(t)$ profile

Mathematical Modeling

The proportionality factor $\alpha(t)$ is defined as the ratio of diluant flow $u(t)$ to permeate flow $q(t)$:

$$\alpha(t) = \frac{u(t)}{q(t)} \tag{1}$$

The change in the feed volume during the operation is given as

$$\frac{dV_f}{dt}(t) = u(t) - q(t) \tag{2}$$

Assuming that the diluant consists of no solutes, the mass balance for the solute concentrations yields

$$\frac{d}{dt} V_f(t) c_{f,i}(t) = -q(t) c_{p,i}(t) \qquad i = 1, 2 \ldots n \tag{3}$$

where $c_{p,i}(t)$ denotes the permeate concentration of solute i at time t.

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Initial Value Problem

Modeling of diafiltration with a system of ODEs:

The volume in the feed tank can be calculated by

$$\begin{cases} \dfrac{dV_f}{dt}(t) = u(t) - q(t) \\ V_f(0) = V_f^0 \end{cases}$$

and the solute concentrations

$$\begin{cases} V_f(t)\dfrac{dc_{f,i}}{dt}(t) = c_{f,i}(t)\left[q(t)\mathcal{R}_i(t) - u(t)\right] \\ c_{f,i}(0) = c_{f,i}^0 \end{cases}$$

where $q(t)$, $\mathcal{R}_i(t)$, $i = 1, 2 \dots n$, are functions of $c_{f,1}(t)$, $c_{f,2}(t) \dots c_{f,n}$, that can be estimated from experimental data or calculated using transfer models.

Analytical solution assuming constant rejections $R_i = \sigma_i$

concentration mode ($\alpha = 0$):

$$c^1_{f,i} = c^0_{f,i} \cdot (N)^{\sigma_i} \quad i = 1, 2 \ldots n \tag{4}$$

constant-volume dilution mode ($\alpha = 1$):

$$c^1_{f,i} = c^0_{f,i} \cdot e^{D(\sigma_i - 1)} \quad i = 1, 2 \ldots n \tag{5}$$

variable-volume dilution mode ($0 < \alpha < 1$):

$$c_{f,i}(t_f) = \frac{c_{f,i}(0)}{\left(1 - \frac{(1-\alpha)V_w}{V_f(0)}\right)^{\frac{\sigma_i - \alpha}{1-\alpha}}} \qquad i = 1, 2. \tag{6}$$

In a more general case:

$$R_i = R_i(c_{f,1}, c_{f,2} \ldots c_{f,n}) \quad i = 1, 2 \ldots n \tag{7}$$

$$q = q(c_{f,1}, c_{f,2} \ldots c_{f,n}) \tag{8}$$

$\hookrightarrow$ Need for numerical technique

Analytical solution assuming constant rejections $R_i = \sigma_i$

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Concentration-(inter)dependent rejection

$$\mathcal{R}_i = \sigma_i \quad \text{or} \quad \mathcal{R}_i = \mathcal{R}_i(c_{f,1}, c_{f,2}) \quad ?$$

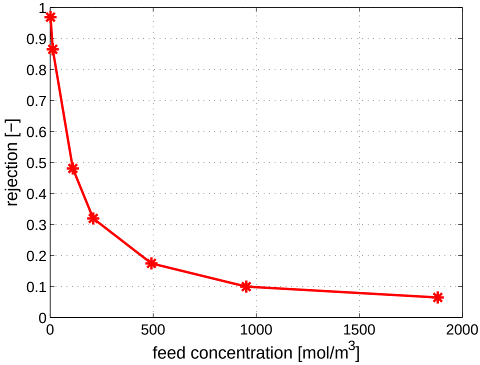


Figure: Rejection of DS-5 NF membrane for NaCl at 30 bar and 25°C

Concentration-(inter)dependent flux

$$q = q(c_{f,1}, c_{f,2})$$

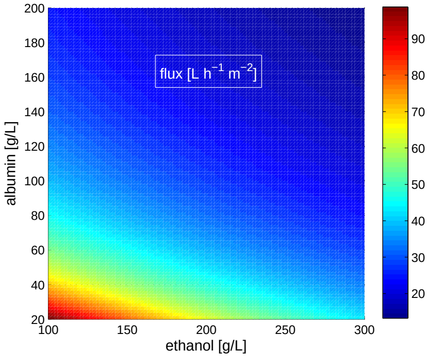
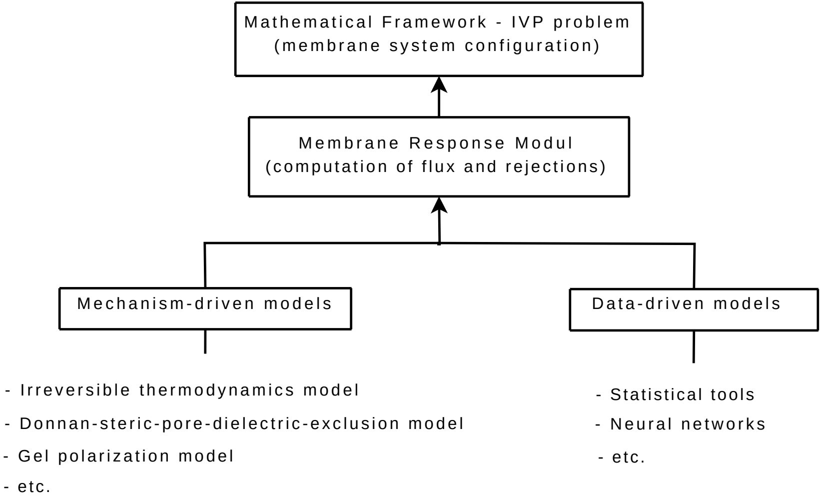


Figure: Influence of feed composition on permeate flux (20 kDa CA membrane, 4 bar) [data taken from: Jaffrin et al. J. Membr. Sci 97 (1994) 71–82]

Flow-chart of the simulation approach



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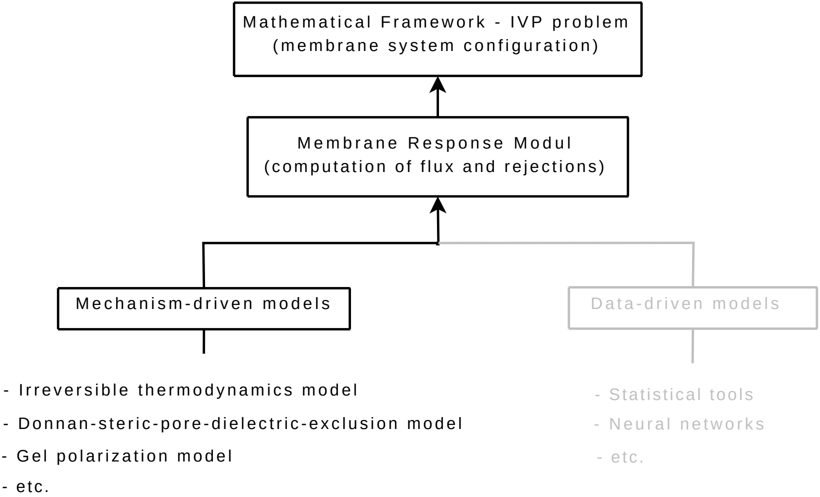

Mechanism-driven models: IT model

Kedem and Katchalsky equations:

$$J = L_p \triangle P - L_p \sigma \triangle \pi \tag{9}$$

$$J_s = P_s \triangle \pi + (1-\sigma) J \bar{c} \tag{10}$$

Symbol	Name	Unity (S.I.)
J	total volume flux	m/s
J_s	molar solute flux	$mol/(m^2\ s)$
$\triangle P$	transmembrane pressure	Pa
$\triangle \pi$	osmotic pressure difference	Pa
$\bar{c}$	mean concentration across the membrane	mol/m^3
L_p	**hydraulic permeability**	m/Pa
σ	**reflection coefficient**	–
ω	**solute permeability coefficient**	$mol/(m^2\ s\ Pa)$

Mechanism-driven models: IT model

Estimate rejection by solving the nonlinear equation:

$$c_{f,i}(t)(1-\mathcal{R}_i(t)) = \frac{\sum_{k=1}^{2} P_{s,k} c_{f,k}(t)\mathcal{R}_k(t)}{L_p\left[\Delta P - RT\sum_{k=1}^{2}\sigma_k \nu_k c_{f,k}(t)\mathcal{R}_k(t)\right]} - (1-\sigma_i)\frac{c_{f,i}(t)\mathcal{R}_i(t)}{\ln(1-\mathcal{R}_i(t))}$$

The permeate flux can be then recovered as:

$$J(t) = L_p\left[\Delta P - RT\sum_{k=1}^{2}\sigma_k \nu_k c_{f,k}(t)\mathcal{R}_k(t)\right].$$

Numerical computation task:

$$\mathcal{R}_i = f(c_{f,1}, c_{f,2}, \triangle P)\big|_{L_{p,k}, P_{s,k}, \sigma_k} \qquad \text{for i=1,2}$$

Mechanism-driven models: DSPM-DE model

The extended Nernst-Planck model:

$$J_{s,j} = -D_{j,p}\frac{dc_j}{dx} - \frac{z_j c_j D_{j,p}}{RT}F\frac{d\psi}{dx} + K_{j,c}c_j\dot{V} \tag{11}$$

The permeate concentration for a 1:1 type electrolyte is given by [Bowen et al., 2002]

$$c_p = \frac{(Pe_1 + Pe_2)c_{av,1}^2 + (Pe_1 + Pe_2)X_d c_{av,1} - (2c_{av,1} + X_d)\Delta c_1}{\left(\frac{Pe_1}{K_{c,1}+\frac{Pe_2}{K_{c,2}}}\right)c_{av,1} + \frac{Pe_1}{K_{c,1}}X_d} \tag{12}$$

Pe_j is the Peclet number

$$Pe_j = \frac{K_{c,j}r_p^2\Delta P_e}{K_{d,j}D_{\infty,j}\eta_0}$$

which depends on the hindrance factors

$$K_{c,j} = (2-\Phi_j)\left(1.0 + 0.054\lambda_j - 0.988\lambda_j^2 + 0.441\lambda_j^3\right)$$
$$K_{d,j} = 1 - 2.30\lambda_j + 1.154\lambda_j^2 + 0.224\lambda_j^3$$

Mechanism-driven models: DSPM-DE model

Numerical computation task:

$$\mathcal{R}_i = f(c_{f,1}, c_{f,2}, \triangle P)\big|_{X_d, r_p, r_j, \epsilon^*, \eta_0, D_{\infty,j}, z_j} \qquad \text{for i=1,2}$$

no direct method to estimate the membrane charge density X_d

- $\hookrightarrow$ depends on the membrane chemistry and on the specific adsorption of ions
- $\hookrightarrow$ estimates based on experimental isotherm data
- $\hookrightarrow$ note analogy to $P_s = P_s^* \left(\frac{c_f}{c_f^*}\right)^m$

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Model Validation

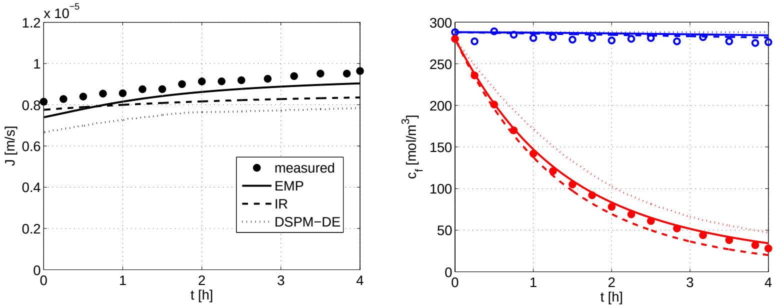

Figure: Validation run no. 1: organics/electrolyte separation, constant-volume dilution mode with pure water as diluant.

[Kovács et al., J. Membr. Sci. 327 (2009) 164–173]

Model Validation

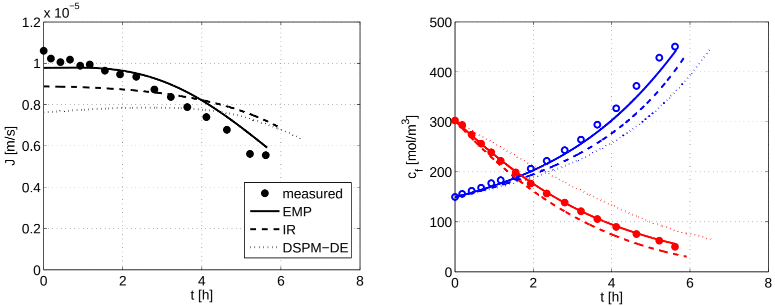

Figure: Validation run no. 2: organics/electrolyte separation, variable-volume dilution mode adjusting the proportionality factor (α) to 0.75 and using pure solvent as diluant

[Kovács et al., J. Membr. Sci. 327 (2009) 164–173]

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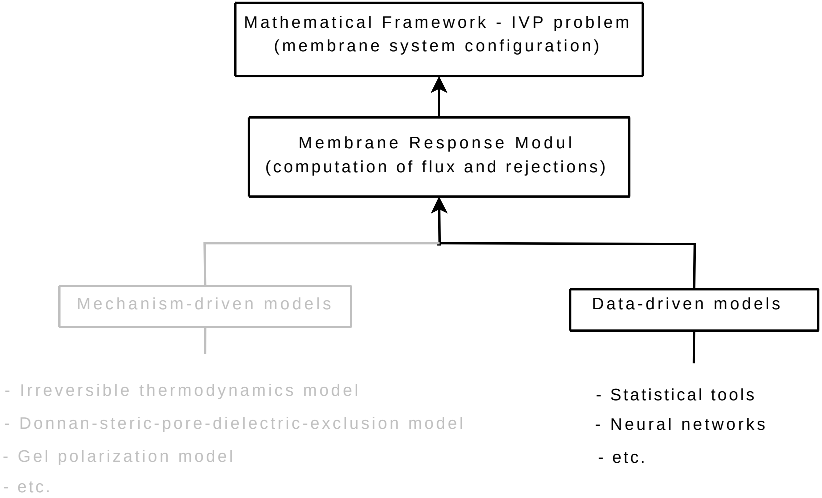

Data-driven modeling approach

Problem statement:

- multi-component systems in real world membrane applications
- information on the composition of the process streams is restricted to the available chemical analysis.
- limited information on several components
- many of the measured quantities are not solute-specific quantities;
- measured quantities represent certain collective features of a group of solutes of common types.

Empirical method as a reasonable alternative over physical models:

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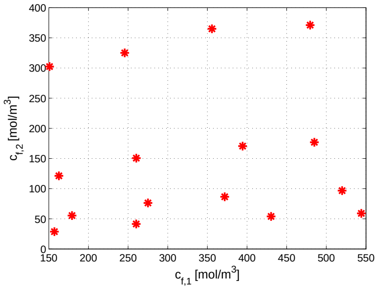
Data-driven modeling approach

Experimental design

Concentrate the initial feed solution, then add pure water to obtain the initial volume, and repeat this procedure several times. $\Rightarrow$ whole range scan, extreme points, evenly distributed data.



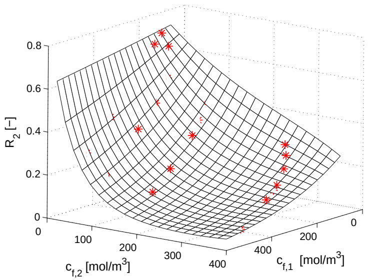


Figure: Map of information.

Data-driven modeling approach

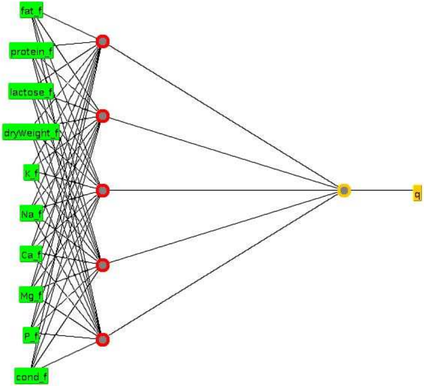
Mathematical tools

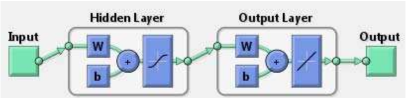
Statistical methods

(cooperative partner: A. Ittzés, Department of Mathematics and Informatics, University of Budapest, Hungary)

Support Vector Machines & Neural Networks

(cooperative partner: M. Grachten, Institute of Psychoacoustics and Electronic Music, University of Ghent, Belgium)





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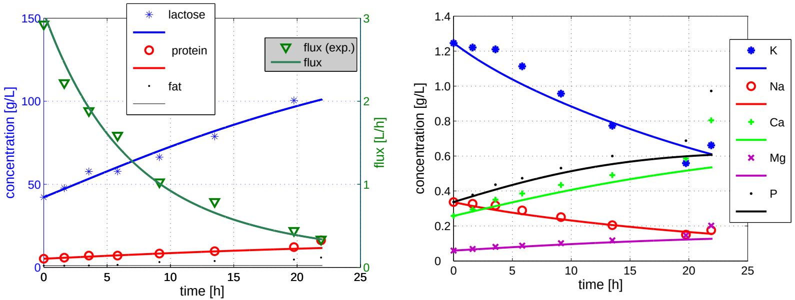
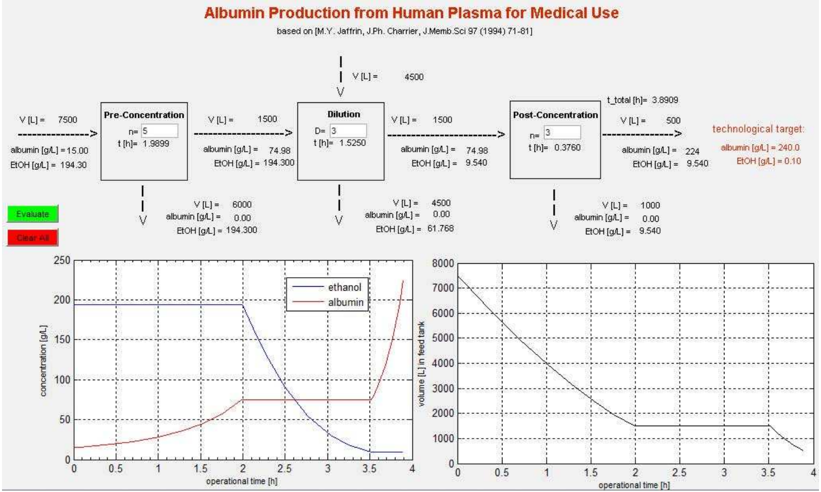


Figure: Partial demineralization and concentration of acid whey with NF (XN45-TriSep, 20 bar, 40^{o}C). Variable volume dilution mode with α=0.75. (Corvinus University of Budapest, Hungary).

[Román et al., J. Food. Process Eng. accepted]

Simulation of multi-step processes



Description of the optimization problem:

Objective function: cost minization $\min_{u(t)} \mathcal{J} = k_1 t_f + k_2 n^{loss} + k_3 V_d$

State variables: $c_{f,1}(t)$, $c_{f,2}(t)$ and $V_f(t)$

Control variable: $u(t)$

Constraints: product quality and technological demands

$$
\begin{aligned}
c_{f,2}(t_f) &\leq \text{const}\\
V_f(t_f) &= \text{const}\\
V_f(t) &\in [\text{lb ub}]\\
u(t) &\in [\text{lb ub}]
\end{aligned}
$$

Dynamic optimization tools:

Determination of optimal control trajectory subject to equality and inequality constraints, using orthogonal collocation on finite elements methods (Dynopt) and control vector parametrization methods (DOTcvp).

M. Čižniar, M. Fikar, M. A. Latifi, MATLAB Dynamic Optimisation Code DYNOPT. User's Guide. Bratislava, (2006)

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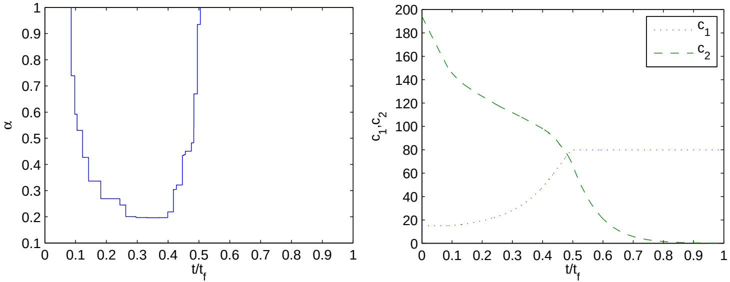

(a) $\alpha(t)$ profile (b) concentration profile

Figure: Illustrative example for optimal trajectories of $\alpha(t)$ and concentrations employing a $40\times$piece-wise constant function.

[Fikar et al., J. Membr. Sci. 355 (2010) 168-174]

Generality versus Specificity

Optimization on a case-by-case basis:

- a *general* methodology for designing DVD process
- a *unique* solution for each application

Output of the optimization depends on:

- membrane response ($\mathcal{R}_i$ and q),
- terms involved in the in the cost function,
- numerical values of the cost factors k_1, k_2, and k_3,
- constraints involved and their numerical values.

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Summary

- A mathematical frame is provided for simulation of batch diafiltration processes.
- Either transport models or real-life experimental data can be employed, without having to modify the governing equations.
- It can be employed for systems where the assumption $\mathcal{R} = \mathrm{const}$ fails.
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Reference I

M. Fikar, Z. Kovács, P. Czermak,
Dynamic optimization of batch diafiltration processes
J. Mem. Sci., 355 (2010) 168–174.

A. Román, Gy. Vatai, A. Ittzés, Z. Kovács, P. Czermak,
Modeling of diafiltration processes for demineralization of acid whey: an empirical approach
J. Food. Process Eng., accepted.

Z. Kovács and M. Discacciati and W. Samhaber,
Modeling of batch and semi-batch membrane filtration processes
J. Mem. Sci., 327 (2009) 164-173.

Z. Kovács and M. Discacciati,
Modelling of multi-step microfiltration process for solvent exchange
Hung. J. Ind. Chem., 36 (2008) 65–69.

M. Čižniar, M. Fikar, M. A. Latifi,
MATLAB Dynamic Optimisation Code DYNOPT
User's Guide. Bratislava, (2006)

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