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MATHEMATICAL MODEL OF VARIABLE VOLUME DIAFILTRATION

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The use of ultrafiltration as a separation technique is frequently accompanied by a diafiltration step to remove microsolutes. There are different ways to combine ultrafiltration and diafiltration to obtain the desired final concentration of components. Variable volume diafiltration is a continuous process in which water is continuously added at a rate less than the permeate flow rate so that the concentration of macrosolute continuously increases, and the final concentrations of macrosolute and microsolute can be reached simultaneously. In this paper a mathematical model of variable volume diafiltration is proposed. The model includes both initial volume and concentration, rejection coefficients, processing time as well as water volume added during diafiltration. The developed model could be served for design and optimization purposes.

Keywords: modeling, ultrafiltration, diafiltration

Introduction

Over two decades ultrafiltration has been recognized as a separation technique to fractionate species according to their size. This technique has several advantages over other separation techniques such as distillation, evaporation solvent extraction, chromatography, etc.

Ultrafiltration is widely used as a separation technique in many different fields such as chemical and biochemical engineering, food processing and pharmaceutical industry. In order to achieve macrosolute–microsolute separation different ultrafiltration processes can be used. The concentration of macrosolute by ultrafiltration is frequently accompanied by a diafiltration step to remove microsolute. It consists of a continuous or discontinuous addition of a pure solvent to retentate feed and can be applied to both batch and continuous ultrafiltration processes.

Both, batch and continuous diafilltration can be performed in different ways. Batch diafiltration can be carried out depending on the way the pure solution is added as a continuous or discontinuous batch diafiltration. On the other hand, continuous diafiltration can be performed as a co-current or counter–current [1] process.

An interesting process in which a pure solvent is continuously added at a rate less than permeate flow rate so that concentration of macrosolute and the removal of impurities occurs simultaneously. was proposed by Jeffrin and Charrier [2]. This way a single diafiltration process with a continuously decreasing volume makes possible that the final concentrations of components are reached simultaneously.

The aim of this work is to develop a process model of a variable volume diafiltration. In the presented model the initial solution concentration, initial volume, retention, processing time as well as the membrane area are included.

This model differs from the approach given by Jaffrin and Charrier [2] where the rejection coefficient was not included. Thus, on the basis of incomplete macrosolute rejection and the constant flux assumption an analytical solution is obtained.

Model

Let us consider the diafiltration process schematically presented in *Fig.1.* The equation of continuity is given by:

$$\frac{dV}{dt} = Q_D - Q_F \tag{1}$$

Here V is the volume of the solution in the tank and Q_D and Q_F are diafiltration water flow rate and filtrate flow rate respectively.

The mass balance of the macrosolute can be written as

$$\frac{d(VC)}{dt} = Q_F C(1-R) \tag{2}$$

Table 1 Values of model parameters and coefficients

Parameter	Unit	Value
A	m^2	1
J	m^3/m^2s	$2.5 \cdot 10^{-5}$
V_0	m^3	0.2
R	1	0.9 -1
r	1	0 – 0.1
C_f/C_0	1	2-10
c_0/c_f	1	2-10
β_{const}	1	variable
β_{var}	1	variable
α	1	variable

where c is concentration, and R is the macrosolute rejection coefficient.

In order to obtain concentrated solution with the final volume V_f the flow rate of diafiltration water must be a constant smaller fraction of Q_F.

$$Q_D = \alpha Q_F \quad \alpha < 1 \tag{3}$$

After rearranging *Eq.(2)* becomes

$$\int_{C_0}^{C_f} d(\ln C) = -\int_0^{t_f} \frac{Q_F(1-R)}{V} dt - \int_{V_0}^{V_f} d(\ln V) \tag{4}$$

From the third term of *Eq.(4)* it follows

$$V = V_0 - Q_F(1-\alpha)t \tag{5}$$

and the first term on the right hand side of *Eq.(4)* becomes

$$-\int_0^{t_f} \frac{Q_F(1-R)}{V} dt = \frac{(1-R)}{(1-\alpha)} \ln\left[1 - \frac{Q_F(1-\alpha)}{V_0} t_f\right] \tag{6}$$

By introducing *Eq.(6)* in *(4)*, it follows

$$\ln\frac{C_f}{C_0} = \frac{(1-R)}{(1-\alpha)} \ln\left(1 - \frac{Q_F(1-\alpha)}{V_0} t_f\right) - \ln\frac{V_f}{V_0} \tag{7}$$

from which the relative concentration of macrosolute can be related with time

$$\frac{C_f}{C_0} = \frac{1}{\left(1 - \frac{(1-\alpha)J \cdot A \cdot t_f}{V_0}\right)^{\frac{R-\alpha}{1-\alpha}}} \tag{8}$$

The processing time necessary to reach the desired final concentration can be calculated as

$$t_f = \left[1 - \left(\frac{C_0}{C_f}\right)^{\frac{1-\alpha}{R-\alpha}}\right] \frac{V_0}{(1-\alpha)JA} \tag{9}$$

The processing time can be related to microsolute concentrations

$$t_f = \left[1 - \left(\frac{c_0}{c_f}\right)^{\frac{1-\alpha}{r-\alpha}}\right] \frac{V_0}{(1-\alpha)JA} \tag{10}$$

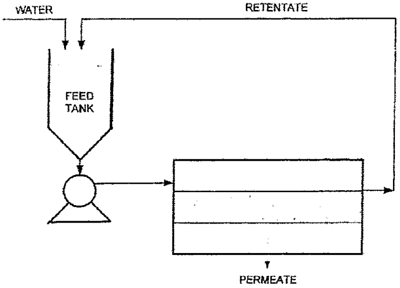

Fig.1 Schematic representation of the variable volume diafiltration process

where r is the microsolute rejection coefficient which is zero or close to zero.

From the last two *Eqs.(9)* and *(10)* the relation between macrosolute and microsolute concentration can be found

$$\frac{c_0}{c_f} = \left(\frac{C_0}{C_f}\right)^{\frac{r-\alpha}{R-\alpha}} \tag{11}$$

The coefficient α can now be calculated from the above *Eq.(11)*

$$\alpha = \frac{r \ln\frac{C_0}{C_f} + R \ln\frac{c_f}{c_0}}{\ln\frac{C_0}{C_f} + \ln\frac{c_f}{c_0}} \tag{12}$$

The solution volume added during the diafiltration in this process is

$$V_{D,\mathrm{var}} = Q_D t = \alpha J A t_f \tag{13}$$

combining with *Eq.(9)* one can get

$$\beta_{\mathrm{var}} = \frac{V_{D,\mathrm{var}}}{V_0} = \frac{\alpha}{(1-\alpha)} \left[1 - \left(\frac{C_0}{C_f}\right)^{\frac{1-\alpha}{R-\alpha}}\right] \tag{14}$$

In the classical (constant volume) diafiltration process the volume ratio is

$$\beta_{const} = \frac{V_{D,const}}{V_0} = \frac{1}{1-r} \ln\frac{c_0}{c_f} \tag{15}$$

where concentration ratio c_f/c_0 can be found from *Eq.(11)*.

Calculation

The calculations of the developed model were carried out on the basis of parameters given in *Table 1*.

The influence of the relative concentration of macrosolute on processing time at different retention are given in *Fig.2*. The calculations were carried out for initial feed volume of $0.2m^3$, and $\alpha = 0.3$. As expected, we have the shortest time at higher retention as it is at batch ultrafiltration [3].

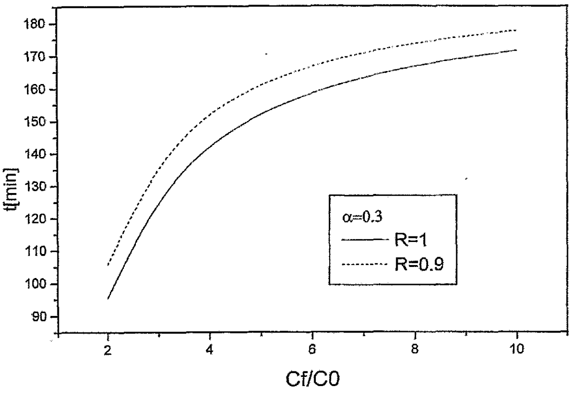

Fig.2 Processing time vs. macrosolute relative concentration

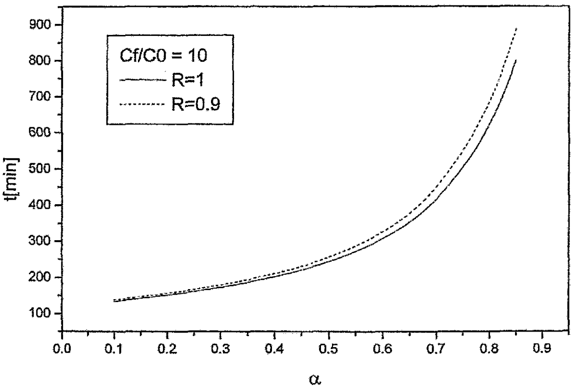

Fig.3 Processing time vs. retentate dilution

Fig.3 shows how processing time depends on the ratio of the dilution flow rate to the permeate flow rate, α, at different retention. It can be seen that the processing time increases with increasing α, and that the value of α over 0.7 leads to very high processing time.

The processing time as the function of the relative dilution of the microsolute at different values of α are shown in *Fig.4*. It should be noted that at $\alpha = 0.3$ the processing time is almost independent of the relative dilution. With increasing an α the processing, time rises significantly with the relative dilution. A simple way of comparing variable volume and constant volume diafiltration is to compare the amount of the diafiltration solvent used to reach desired the final concentration.

The results of the calculation on *Fig.5* represent the relative volume of the water added during the constant volume and variable volume diafiltration. It is important to note that the variable volume diafiltration requires less diluent water than the constant volume diafiltration.

Conclusions

A more realistic model which differs from Jaffin and Charrier`s [2] and includes the rejection coefficient is presented. The model provides the basis for more complex simulations of variable volume diafiltration and can be useful in analysis of process parameters. The obtained analytical solution enables simple calculations such as processing time, amount of diafiltration solvent, concentration of macrosolute and dilution of microsolute. The calculations also show that variable volume diafiltration needs less diafiltration liquid than the constant volume diafiltration which could be of practical interest.

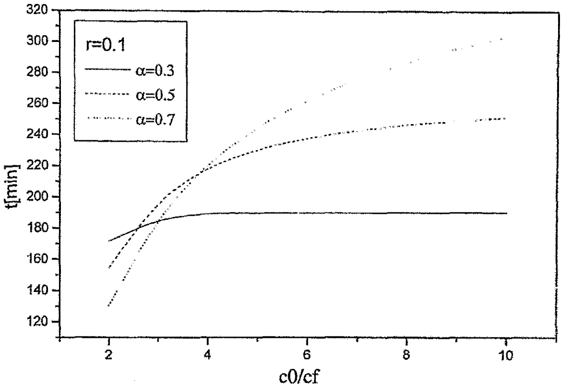

Fig.4 Processing time vs. relative microsolute dilution

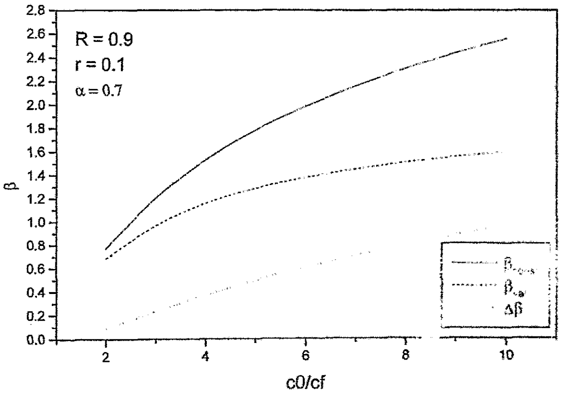

Fig.5 Relative diafiltration volume vs. microsolute dilution at the process with constant and variable volume diafiltration

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SYMBOLS

A	membrane area, m^2
C	concentration of macrosolute in any time, wt.%
C_0	initial concentration of macrosolute , wt.%
C_f	final concentration of macrosolute wt.%
c_0	initial concentration of microsolute , wt.%
c_f	final concentration of microsolute wt.%
J	permeate flux, m^3/m^2s
Q_D	water (solution) flow rate added during diafiltration, m^3/s
Q_F	filtration flow rate, m^3/s
R	macrosolute rejection coefficient
r	microsolute rejection coefficient
V	volume in the tank, m^3
V_0	initial volume, m^3
V_f	final volume, m^3
t	time, s
t_f	final time, s
α	defined by *Eq.(3)*

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