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NOTE

Mathematical Simulation for Membrane Filtration Systems

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Abstract

Time variation in filtration systems variables, e.g., concentrations, volume, and permeation rate, is mathematically simulated. Rigorous mathematical solutions are illustrated for a physical model with stepwise approximation. A detailed setup for numerical calculations is given.

In designing a membrane filtration system, we usually strive for the most economical and optimal system design. This involves a compromise between many operation parameters, such as membrane area, circulation rate, rate of permeate and concentrate withdrawal, and amount of recycle. Experimentally, measurement of such changes is extremely time consuming and in many situations it is desirable to predict the performance of a proposed system and to make adjustments in operating parameters prior to finalizing design and operation. The objective of this paper is to present a mathematical solution for simulating a membrane process which can be handled by computer calculation. There is a pressing need for such a solution, and its presentation should help to eliminate repetitive pilot studies in membrane filtration and related systems. Mathematical simulation of the concentration process as a function of time can be set up from a set of mass balance equations. The closed form solution of the equations can be obtained, assuming that the concentrations are the only variables. However, in practice, other variables such as membrane characteristics do change with concentration, thus introducing the cross-term difficulty in solving the equations. There are two methods to get around the problem. One is applying mathematical approximations to a rigorous physical model, the other is to construct an approximate physical model and give a rigorous mathematical solution. Due to mathematical complexity, the physical implication in the first approach is not always clear, and the approximation may not be applicable in some boundary conditions. This note presents an analysis using the second approach.

The method of constructing an approximate physical model involves a stepwise variation of selected variables. During the concentration process, at a small time interval, these variables are assumed constant. At the beginning of each successive time interval the variables are updated to reflect changes which would have occurred during the previous time interval. Such approximations are predictable, and close to exact solutions can be obtained if sufficiently small incremental steps are chosen such that further decrease in stepwidth does not significantly affect the result. An example of waste oil concentration system is given below.

Referring to Fig. 1, this membrane filtration system consists of a holding bath B and a membrane loop L. Concentrate is being circulated within the loop and also recycled to the holding bath. Permeate is withdrawn. The following nomenclature is used:

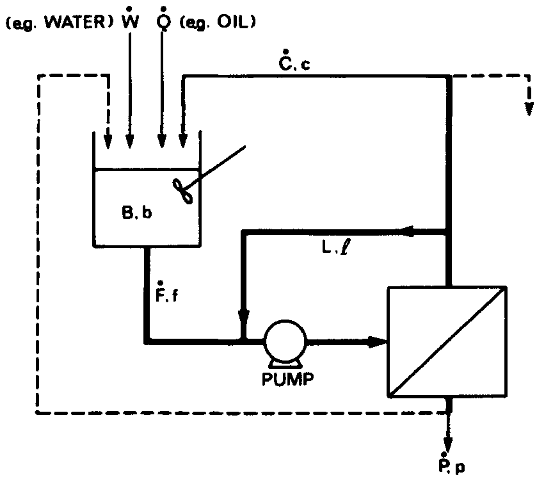

FIGURE 1.

$\dot{W}$	rate of solvent added to the bath, e.g., water
$\dot{Q}$	rate of suspended material added to the bath, e.g., oil
B	volume of the suspension in the bath, e.g., oil emulsion
b	% concentration of suspended material in the bath
$\dot{F}$	rate of the feed to the membrane loop
f	% concentration of the feed
$\dot{C}$	rate of recycle of the concentrate
c	% concentration of the concentrate
L	volume of the loop
l	% concentration of the loop content
$\dot{P}$	rate of withdrawal of the permeate
p	% concentration of permeate
$x(t) = dl/dt$	rate of change of loop concentration
$z(t) = db/dt$	rate of change of bath concentration
R	rejection constant of the membrane
t	time

Mass balance equations are set as follows: At a small time interval, B and $\dot{P}$ are assumed constant. The assumption of B = constant is achieved by physically adding additional solvent to the bath at a rate of $\dot{W}'$:

$$\dot{W}' + \dot{W} + \dot{Q} + \dot{C} = \dot{F} \tag{1}$$

$$B\frac{db}{dt} + \dot{F}f = \dot{Q} + \dot{C}c \tag{2}$$

$$\dot{F} = \dot{C} + \dot{P} \tag{3}$$

$$\dot{F}f - \dot{P}p - \dot{C}c = L\frac{dl}{dt} \tag{4}$$

For the nth concentration step starting from $t = t_{n-1}$, $l = l_{n-1}$, $b = b_{n-1}$ to $t = t_n$, $l = l_n$, $b = b_n$, we have

$$b_n = b_{n-1} + \int_0^{\Delta t} z\,dt \tag{5}$$

$$l_n = l_{n-1} + \int_0^{\Delta t} x\,dt \tag{6}$$

$$p_n = (1 - R)l_n \tag{7}$$

Substitute

$$H = \dot{C}l_{n-1} + \dot{Q} - \dot{F}b_{n-1} \tag{8}$$

$$D = \dot{C} \tag{9}$$

$$E = \dot{P}(1 - R) + \dot{C} \tag{10}$$

$$G = l_{n-1}\{\dot{P}(1 - R) + \dot{C}\} - \dot{F}f_{n-1} \tag{11}$$

and from Eq. (3)

$$\dot{F} = \dot{C} + \dot{P}$$

Assuming good mixing, then $f = b$ and $c = l$. Combining the above, at any time $t = t_n$, we have

$$Bz + \dot{F}\int_0^{\Delta t} z\,dt = H + D\int_0^{\Delta t} x\,dt \tag{12}$$

$$\dot{F}\int_0^{\Delta t} z\,dt = E\int_0^{\Delta t} x\,dt + G + Lx \tag{13}$$

Equations (12) and (13) can be solved by Laplace transform. Thus

$$Z(s) = \frac{H + DX(s)}{Bs + \dot{F}} \tag{14}$$

$$\dot{F}Z(s) = (Ls + E)X(s) + G \tag{15}$$

Solving simultaneous Eqs. (14) and (15), we have

$$X(s) = \frac{K_1}{(s + r_1)} + \frac{K_2}{(s + r_2)} \tag{16}$$

$$Z(s) = \frac{K_3}{(s + r_3)} + \frac{K_4}{(s + r_1)} + \frac{K_5}{(s + r_2)} \tag{17}$$

By invert Laplace transform, we obtain the solutions

$$x(t) = K_1e^{-r_1t} + K_2e^{-r_2t} \tag{18}$$

$$z(t) = K_3e^{-r_3t} + K_4e^{-r_1t} + K_5e^{-r_2t} \tag{19}$$

then

$$\int_0^{\Delta t} x\,dt = \frac{K_1}{r_1} + \frac{K_2}{r_2} - \left(\frac{K_1}{r_1}e^{-r_1t} + \frac{K_2}{r_2}e^{-r_2t}\right) \tag{20}$$

$$\int_0^{\Delta t} z\,dt = \frac{K_3}{r_3} + \frac{K_4}{r_1} + \frac{K_5}{r_2} - \left(\frac{K_3}{r_3}e^{-r_3t} + \frac{K_4}{r_1}e^{-r_1t} + \frac{K_5}{r_2}e^{-r_2t}\right) \tag{21}$$

where

$$K_1 = \frac{(\dot F H - \dot F G)/BL + r_1 G/L}{r_2 - r_1} \tag{22}$$

$$K_2 = \frac{(\dot F H - \dot F G)/BL + r_2 G/L}{r_1 - r_2} \tag{23}$$

$$K_3 = \frac{H}{B} + \frac{K_1 D/B}{r_1 - \dot F/B} + \frac{K_2 D/B}{r_2 - \dot F/B} \tag{24}$$

$$K_4 = \frac{(D/B)K_1}{(\dot F/B) - r_1} \tag{25}$$

$$K_5 = \frac{(D/B)K_2}{(\dot F/B) - r_2} \tag{26}$$

$$r_1 = \frac{BE + \dot F L}{2BL} + \frac{1}{2}\sqrt{\left(\frac{BE + \dot F L}{BL}\right)^2 - 4\left(\frac{E\dot F - \dot F D}{BL}\right)} \tag{27}$$

$$r_2 = \frac{BE + \dot F L}{2BL} - \frac{1}{2}\sqrt{\left(\frac{BE + \dot F L}{BL}\right)^2 - 4\left(\frac{E\dot F - \dot F D}{BL}\right)} \tag{28}$$

$$r_3 = \frac{\dot F}{B} \tag{29}$$

To compensate the change of $\dot P$ and B and the addition of $\dot W'$, they are adjusted before every concentration step. The adjusted values are $\dot P'$ and B'. The value of $\dot P$ as a function of l can be obtained from experimental data. $\dot P'$ is taken from the experimental $\dot P$ value at the average of the initial and final l concentrations in a concentration step in the approximation. Since the final concentration is not known beforehand, an iteration process is needed. However, if $\dot P$ is a smooth function of l, $\dot P'$ can be chosen at a compensated value estimated from the knowledge of the previous step. If the stepwidth is small, the error would be insignificant. B is a function of time and can be compensated for by withdrawing the additional solvent from the bath at the beginning of the nth step in the amount of $\dot W'\Delta t$. Thus the setup for the numerical calculation is

$$b_1 = \left(b_0' + \int_0^{\Delta t} z\,dt\right) \quad \text{using } \dot P = \dot P_0,\ B = B_0' \tag{30}$$

$$b_n = \left(b_{n-1}' + \int_0^{\Delta t} z\,dt\right) \quad \text{using } \dot P = \dot P_{n-1}',\ B = B_{n-1}' \tag{31}$$

$$l_n = l_{n-1} + \left(\int_0^{\Delta t} x\,dt\right) \qquad \text{using } b = b'_{n-1},\ \dot{P} = \dot{P}'_{n-1},\ B = B'_{n-1} \tag{32}$$

where

$$\dot{P}'_1 = \dot{P}_0 - 2(\dot{P}_0 - \dot{P}_1) \tag{33}$$

$$\dot{P}'_{n-1} = \dot{P}'_{n-2} - 2(\dot{P}'_{n-2} - \dot{P}_{n-1}) \tag{34}$$

$$B'_0 = B_0 - \dot{W}'\Delta t/2 = B_0 - (\dot{P} - \dot{W} - \dot{Q})\Delta t/2, \qquad b'_0 = \frac{b_0 B_0}{B'_0} \tag{35}$$

and

$$B'_{n-1} = B'_{n-2} - \dot{W}'\Delta t = B'_{n-2} - (\dot{P} - \dot{W} - \dot{Q})\Delta t, \qquad b'_{n-1} = \frac{b_{n-1}B'_{n-2}}{B'_{n-1}} \tag{36}$$

Here again the subscript $n - 1$ denotes the initial and n denotes the final points of a concentration step.

A comparison of experimental and calculated results is depicted in Fig. 2. Experimentally determined, $R = 99\%$ and $\dot{P}s$ as a function of l at given conditions (40°C, 20 psi, 268 m/min cross-flow velocity) for a 0.01197 m^2 membrane in oil–emulsion filtration, as shown in Fig. 2, are used as input data. Other input data used are: $\dot{W} = 11$ ml/min, $\dot{Q} = 0$, $\dot{C} = 0$, $L = 200$ ml, $B_0 = 3000$ ml, $b_0 = l_0 = 0.2\%$. The time interval $\Delta t = 1$ min is used in the calculation.

A system where the permeate is recycled and the concentrate is withdrawn is illustrated by the dashed line in Fig. 1. This configuration is found where permeate is recovered as wash solvent. The mathematical solution is a symmetry case to the above example. The necessary changes include the interchange of $\dot{C}$ and $\dot{P}$, c and p in Eqs. (1) to (4), (35), and (36), and interchange of $\dot{C}$ and $\dot{P}(1 - R)$ in Eqs. (8) and (9). In this system a steady-state condition can be reached if

$$\dot{W} + \dot{Q} + \dot{P} = \dot{F}, \qquad \dot{C} = \dot{W} + \dot{Q}, \qquad p = l_s(1 - R)$$

then

$$b_s = \frac{\dot{Q} + \dot{P}p_s}{\dot{W} + \dot{Q} + \dot{P}} \qquad \text{and} \qquad \dot{C} = \frac{\dot{Q}}{c_s}$$

where subscript s denotes steady state.

The membrane area needed can be calculated from the permeation rate $\dot{P}$ obtained from the preset b_s, $\dot{Q}$, $\dot{W}$, c_s, and R.

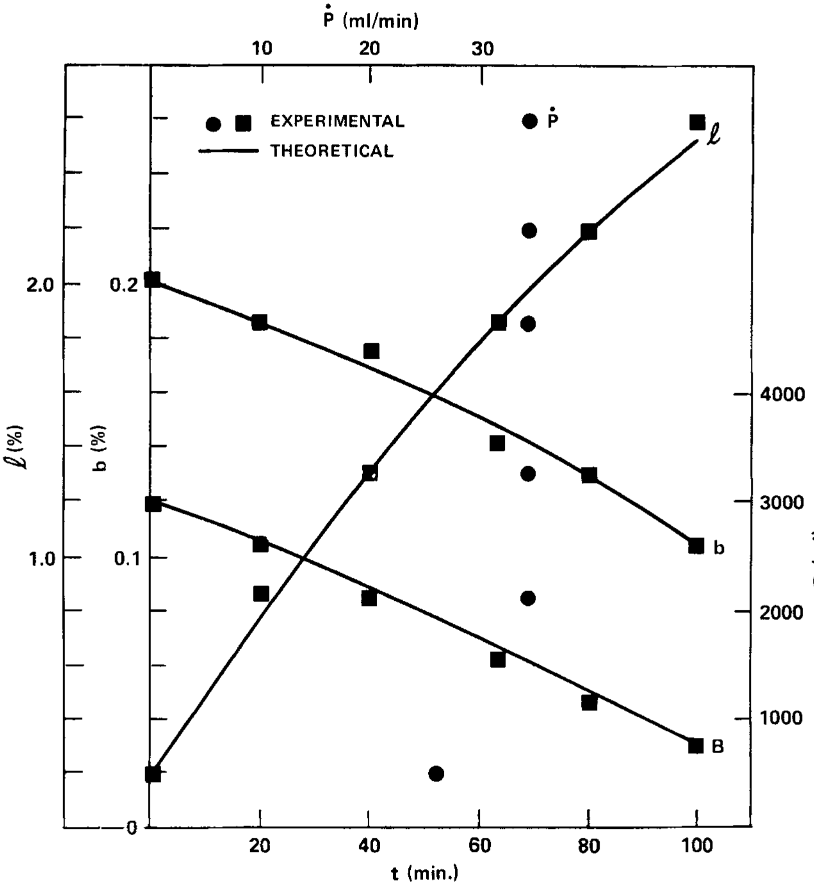
Ṗ (ml/min)
10
20
30
● ■ EXPERIMENTAL
——— THEORETICAL
● Ṗ
ℓ
b
B
ℓ (%)
b (%)
2.0
1.0
0.2
0.1
0
4000
3000
2000
1000
B (ml)
20
40
60
80
100
t (min.)

FIGURE 2.

Mathematical solutions for other variations of the system have been derived similarly. In general, the number of concentration variables in the whole system governs the degree of simultaneous equations involved in the Laplace transform.

For all the above numerical calculations, computer programs have been written (*1*).

REFERENCE

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