NUMERICAL SOLUTION OF ELECTROKINETICS MASS TRANSFER MODEL FOR PROTEIN RECOVERY THROUGH MEMBRANE ELECTROFILTER

Syaubari and S. Nurdin[*)]

Abstract

Separation based on electrophoresis and electroosmosis (electrokinetics) of binary mixture of proteins (bovine serum albumin – hemoglobin) was studied on an membrane electrofilter. The mixture was separated using ionic polycarbonate membrane with variable studied consist of voltage, current, protein diffusivity, and electrophoresis mobility. Operation parameters were varied to investigate hemoglobin concentration, which pass semi permeable membrane. A model has been derived based on mass transfer principle for the case of unsteady state. For simplification, the model has been modified using Cramer Method with pseudo steady state approach to give the dimensionless form. A program for computer simulation has been written in C/C++ language. This programming language was shown to have more effective computing ability. Furthermore, using the model and simulation on computer, the result indicates that initial mechanism of electrofilter important variables were electroosmosis and electrophoresis mobility. In addition, the electrofilter can also be used to separate and to concentrate protein on their buffer solution.

Keywords: *electrophoresis; electroosmosis; protein; membrane; electrofilter*

Abstrak

*Penelitian pemisahan yang didasarkan pada elektroforesis dan elektrosomosis (elektrokinetik) campuran biner protein (*bovine serum albumin – hemoglobin*) ini dilakukan pada elektrofilter membran. Campuran dipisahkan menggunakan membran polikarbonat ionik dengan variabel voltase, arus, difusifitas protein dan mobilitas elektroforesis. Parameter operasi divariasikan untuk mengamati konsentrasi hemoglobin melalui membran semipermeabel. Model diturunkan berdasarkan prinsip transfer massa untuk kasus tak mantap. Untuk penyederhanaan, model dimodifikasi menggunakan metode Cramer dengan pendekatan* pseudo steady state *untuk memberikan bentuk tak berdimensi. Program simulasi komputer ditulis dalam bahasa C/C++. Bahasa pemrograman ini menunjukkan kemampuan perhitungan yang lebih efektif. Selanjutnya, dengan menggunakan model dan simulasi pada komputer, hasilnya menunjukkan bahwa variabel penting dari mekanisme awal elektrofilter adalah mobilitas elektroosmosis dan elektroforesis. Selain itu, elektrofilter dapat juga digunakan untuk memisahkan dan mengkonsentrasikan protein pada larutan buffer.*

Kata kunci: *elektroforesis; elektroosmosis; protein; membran; elektrofilter*

Introduction

Membrane has been known to use as a potential filter which is able to pass molecules selectivity by size. In the present study, separation of binary mixture of protein was studied using an membrane electrofilter. The mixture was bovine serum albumin –hemoglobin, the separation is useful in terms of hemoglobin recovery. As well known, hemoglobin is one of important components present in human blood. It recovery help people with blood related diseases.

In many cases, the separation achieved by electrophoresis through a membrane is too small to be of interest. To enhance the separation, it has been suggested to use a convective flow counteracting to the electrophoretic motion. Such a method is largely unstudied but seems feasible on a large scale (Lauer and Manigill, 1986).

The approach taken in the work reported in this paper was to use a negatively charged membrane (Mulder, 1991). The generated countercurrent flow was the electroosmotic one. Although the previous discussion suggests that large scale membrane electrofiltration is feasible, little is known about how it can be effectively scaled-up (Wheelwrigth, 1989). Following a brief explanation of the basic separation mechanisms, proof of principle experiments in a membrane electrofiltration device was discussed

[*)] Chemical Engineering Department, Engineering Faculty
Syiah Kuala University, Banda Aceh 23111
E-mail : Syaub@yahoo.com

(Syaubari and Tri, 1995). A mathematical model based on the rate process will be developed and finally used to simulate the performance of the membrane electrofiltration device.

Modelling

General equation of mass transfer through membrane pore could be arranged based on control volume of mass balance between x and x+Δx as shown in Figure 1. The following assumptions are applied:

1. Surface area of membrane is constant (A)
2. Fluxes of the volume is constant (J_v)
3. Solute diffusivity (D) and electrophoresis do not depending on concentration
4. Protein-protein and protein-membrane interaction are neglected
5. Mass transfer direction only to one dimension, dC/dy = 0; and dC/dz = 0.

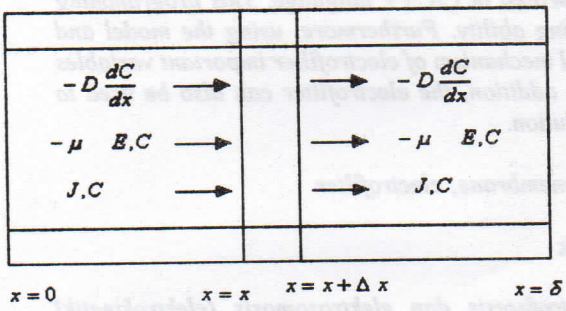

Figure 1. Scheme of mass transfer through membrane pore

Based on Figure 1, mass balance for solute on transient condition can be written as follows :

$$A\Delta x\frac{\partial C}{\partial t}=AJ_vC|_{x=x}-AJ_vC|_{x=x+\Delta x}+\left\{-AD\frac{dC}{dx}\Big|_{x=x}-\left(-AD\frac{dC}{dx}\Big|_{x=x+\Delta x}\right)\right\}+\left\{-A\mu_sE_mC|_{x=x}-\left(-A\mu_sE_mC|_{x=x+\Delta x}\right)\right\} \quad (1)$$

Mass transfer model were developed to separate two proteins on batch operation of electrofilter and using permeable membrane based on negative charge of protein mixture. Electrolyte solutions, which fill membrane pore, were ionized to anion and cation. The cation then moved to pore wall. If pore are contacted with electricity current, the solution closed to wall are rich of positive charge that will move to cathode, but the solution were complicated to move because of closely ions. Meanwhile anion charge moved to anode. This moving will be blocked by solution on pore, therefore, overall solution will move to cathode. It is shown that direction of electro osmosis is countercurrent with electrophoresis. Electro osmosis will occur in cathode chamber and electrophoresis in anode chamber with fast and slow mobility proteins. Resultant of two directions will show that mobility of protein either to anode or to cathode.

To develop mass balance on transient condition for electrofilter process, the following assumptions were considered:

1. Homogenous solution on both chamber will be obtained.
2. Membranes have pore size and potential zeta not depending on membrane position
3. Potential electricity gradient along membrane pore is constant
4. Electrolyte solution as a good buffer
5. On initial condition, homogenous concentration in all position (first chamber, along membrane pore, and second chamber).
6. Polarization of concentration was neglected

Mass balance equation on transient condition for electro filter process can written as follows:

$$V_1\frac{dC_{i,1}}{dt}+V_2\frac{dC_{i,2}}{dt}+A\varepsilon\int_0^t\frac{\partial C_{i,m}}{\partial t}dx=0 \quad (2)$$

Equation (2) shows that concentration change on first and second chamber and along membrane pore were complementary, therefore it will not change protein mass.

Mass transfer along membrane is:

$$\frac{\partial C_{i,m}}{\partial t}=\frac{\partial}{\partial x}\left\{\left(\mu_{osi}E_m-\mu_{efi}E_m\right)C_{i,m}-D_j\frac{\partial C_{i,m}}{\partial x}\right\} \quad (3)$$

or it could be written as

$$\frac{\partial C_{i,m}}{\partial t}=-\alpha_i\frac{\partial C_{i,j}}{\partial x}+D\frac{\partial^2C_{i,j}}{\partial x^2} \quad (4)$$

where

$\alpha_i=(\mu_{eo}-\mu_{efi})E_m$

and the initial value and boundary conditions are

$t=0\Rightarrow C_{i,1(0)}=C_{i,2(0)}=C_{i,m(x,0)}=C_0$

$x=0\Rightarrow V_1\frac{\partial C_{i,1}}{\partial t}=-\alpha_iA\varepsilon C_{i,1}+DA\varepsilon\frac{\partial C_{i,1}}{\partial x}$

$x=L\Rightarrow V_2\frac{\partial C_{i,2}}{\partial t}=-\alpha_iA\varepsilon C_{i,2}+DA\varepsilon\frac{\partial C_{i,1}}{\partial x}$

To simplify the equation, equation (4) will be written in dimensionless form.

$$\frac{\partial\psi_{i,j}}{\partial t}=-\left[\frac{\alpha_i}{\alpha_1}\right]\frac{\partial\psi_{i,j}}{\partial\zeta}+\left[\frac{D_1}{\alpha_1L}\right]\frac{\partial^2\psi_{i,j}}{\partial\zeta^2} \quad (5)$$

or

$$\frac{\partial\psi_{i,j}}{\partial t}=-\beta_1\frac{\partial\psi_{i,j}}{\partial\zeta}+\frac{1}{P_{el}}\frac{\partial^2\psi_{i,j}}{\partial\zeta^2} \quad (6)$$

Where:

$$\psi_{i,j} = \frac{C_{i,j}}{C_o} \qquad \tau = \frac{\alpha t}{L} \qquad \zeta = \frac{x}{L}$$

By applying pseudo steady state approach the equation (6) become

$$\frac{d^2\psi_{i,1}}{d\zeta^2} - P_{ei}\beta_i \frac{d\psi_{i,j}}{d\zeta} = 0 \qquad (7)$$

General solution of equation (7) is:

$$\psi_{i,j} = A + Be^{m_i\zeta} \qquad (8)$$

where

$$m_i = P_{ei} = A + \beta_i$$

Using Cramer Method to the solution of equation (8) were obtained as follows:

$$\psi_{i,1}^{L} = \partial_1 + (1-\partial_1)e^{-\alpha\tau} \qquad (9)$$

and

$$\psi_{i,2}^{R} = \partial_2 + (1-\partial_2)e^{-\alpha\tau} \qquad (10)$$

where

$$\alpha = \frac{\beta_i\left(e^{m_i}+1\right)}{\gamma^*\left(e^{m_i}-1\right)} \; ; \; \partial_1 = \frac{2}{\left(e^{m_i}+1\right)} \; ; \; \partial_2 = \frac{2e^{m_i}}{\left(e^{m_i}+1\right)}$$

$$m_i = \frac{\alpha_i L}{D_i}\beta_i \; ; \; \gamma^* = \frac{V}{AL\varepsilon}$$

Experimental set up

The experimental apparatus is shown in Figure 2. The binary proteins mixture were filled in feeding chamber and buffer of Sodium dihydrogen phosphate and disodium hydrogen phosphate were filled in buffer chamber. Cooling of recycled protein solution was done up to temperature of 4°C. The variation of voltage and current was obtained by adjustment on the power supply panel.

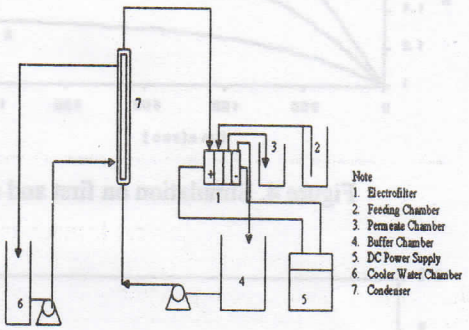

Figure 2. Experimental apparatus set up.

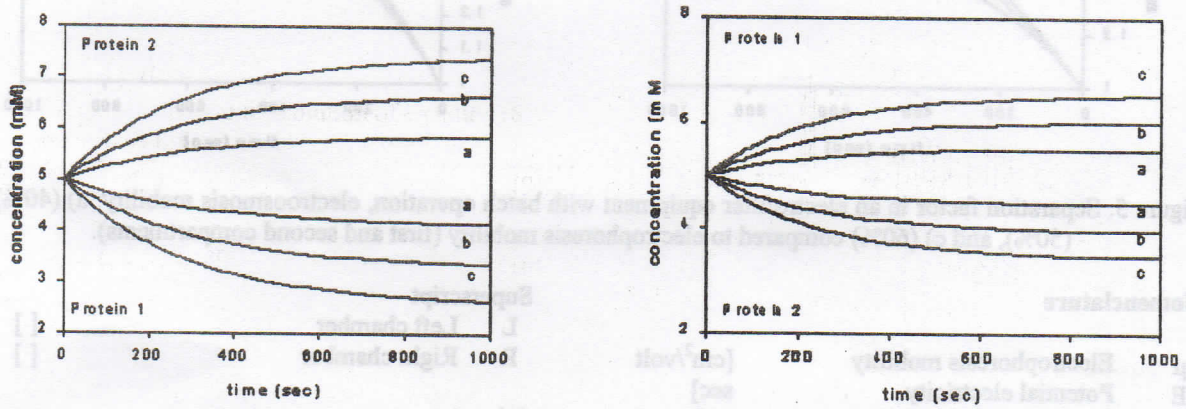

Figure 3. Simulation on first (left) and second (right) compartment with a: 200 Volt; b: 400 Volt and c: 600 volt

Result and discussion

The simulation results using C/C++ language for voltage study are shown on Figure 3,4, and 5. Separation between hemoglobin and bovine serum albumin occurred because of protein mobility in countercurrent direction and membrane as a filter media. Protein 2 is rich on first compartment. Protein movement is relatively fast on first treatment in both compartments. Concentration of protein 1 on first compartment will be minimized and maximized on second compartment by time. Simulation on Figure 3 and Figure 4 shown that the voltage affected the process is in linear factor. It means increase in voltage resulted in an increase in concentration ratio separation protein.

Figure 5 shows that an increase in electrophoresis protein mobility improved separation factor. The effect of electroosmosis and electrophoresis ratio show that on 40% ratio protein 2 is highest in first compartment compared to second compartment due to protein 2 more netto negative than protein 1

Conclusion

The proposed model on protein separation on electrofilter can explain the mechanism of mass transfer of binary protein mixture and predict the dynamic behavior of separation process operating in batchwise. Using the model and simulation on computer, the result indicates that initial mechanism of electrofilter important variables were electroosmosis and electrophoresis mobility. In addition, the electrofilter can also be used to separate and to concentrate protein on their buffer solution.

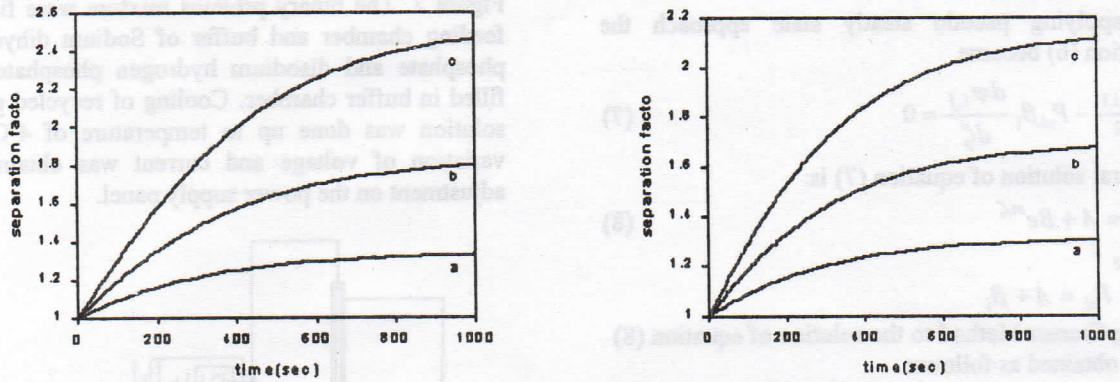

Figure 4. Simulation on first and second compartments for studying separation factor.

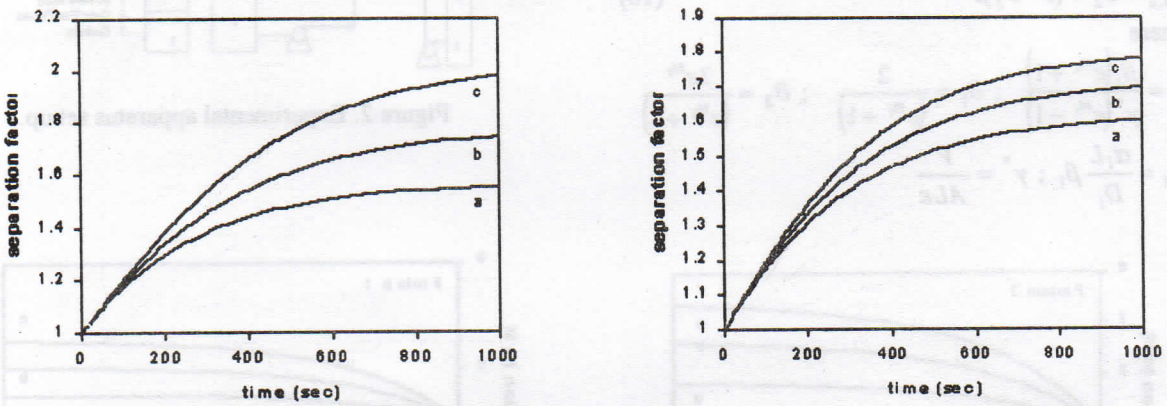

Figure 5. Separation factor in an electrofilter equipment with batch operation, electroosmosis mobility: a) (40%), b) (50%), and c) (60%) compared to electrophoresis mobility (first and second compartments).

Nomenclature

μ	Electrophoresis mobility	[cm^2/volt
E	Potential electricity	sec]
A	Surface area of membrane	[volt/cm]
D_i	Diffusivity of Protein	[cm^2]
V	Volume chamber	[cm^2/sec]
$\psi_{I,j}$	Concentration comparison of	[cm^3]
P_{ei}	component (i) and chamber (j)	[ ]
β_i	Peclet Number	[ ]
γ	Time, was need protein 1 to pass membrane under	[ ]
ζ	electrokinetics effect.	[ ]
L	Geometric factor	[ ]
C	Potential zeta	[cm]
ε	Membrane thickness	[mM]
α	Concentration	[ ]
F	Ratio volume of membrane pore	[cm/sec]
t	Resultant of electrophoresis	[g/sec cm^2]
P	mobility	[sec]
J_v	Flukes	[g/sec cm
	Time	volt]
	Permeability	[cm^3/sec
	Flukes Volume	cm]

Superscript

L	Left chamber	[ ]
R	Right chamber	[ ]

Subscript

i	Protein	[ ]
j	Chamber	[ ]

Literature

Lauer, H.H., and D. Mc Manigill, (1986). "Capillary Zone Electrophoresis in Open Tubular Glass Capillaries", *Anal. Chem.*, 58, 166.

Mulder, M., (1991). "*Basic Principles of Membrane Technology*" Kluwer Academic Publisher, London.

Syaubari and Tri, P.A., (1995), "Kajian Awal Kelakuan Dinamika Proses Pemisahan Protein dengan Alat Electrofilter", *Master Thesis*, ITB, Bandung

Wheelwrigth, S. M., (1989), "The Design of Downstream Process for Large Scale Protein Purification", *Journal of Biotech.*, Vol. 11, 89-102