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MATHEMATICAL MODELING OF MASS TRANSFER
IN A HOLLOW FIBER DIALYZER

BY
TZYY-KAI YU

A THESIS
PRESENTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE
OF
MASTER OF SCIENCE IN CHEMICAL ENGINEERING
AT
NEW JERSEY INSTITUTE OF TECHNOLOGY

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Newark, New Jersey
1983
APPROVAL OF THESIS
MATHEMATICAL MODELING OF MASS TRANSFER
IN HOLLOW FIBER DIALYZER
BY
TZYY-KAI YU
FOR
DEPARTMENT OF CHEMICAL ENGINEERING
BY
FACULTY COMMITTEE

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ABSTRACT

A mathematical model describing the flow characteristics and mass transfer has been developed for the hollow fiber dialyzer in countercurrent dialysis.

The theoretical expressions are developed from a typical Graetz problem for the stream side, and a first order differential equation for the dialyzate side. The solution of the dimensionless concentration profile is obtained as a summation of orthogonal eigenfunctions in closed form, which are given as product of an exponential function and a confluent hypergeometric function.

The analytical solution of the model has been examined by adjusting system parameters, like Sherwood number, Peclet number and the geometry of the system. As expected, at higher Peclet number the bulk concentration in the stream outlet decreases, whereas at higher Sherwood number and higher L/R ratio the bulk concentration increases. This can be used to optimize dialyzer performance.
ACKNOWLEDGMENTS

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CHAPTER ONE
INTRODUCTION

Liquid-phase membrane separation process (such as dialysis, reverse osmosis and ultrafiltration) utilize the difference in the membrane permeability of molecules as a basis for separation. In dialysis, the flux of sloutes across a membrane is mainly controlled by diffusional transport. Large surface area membrane modulus such as hollow fibers unit are often used to compensate for the slow diffusion-controlled flux. Hollow fiber dialyzer has been successfully used, for example, in artificial kidney hemodialysis to remove membrane-permeable waste materials from the blood.

It has been found that the major technical problem of dialysis is to provide a large effective mass transfer surface with adequate mechanical support and uniform flow distribution at acceptable pressure drops and costs. Before these problem can be investigated in a meaningful way, a semiquantitative description of the convection mass transfer taking place will be provided.

The objective of this investigation is to present an analytical solutions which describe the flow characteristics and the mass transfer of a boundle of hollow fibers in
countercurrent dialysis.

In this thesis, a general analytical solution of a mathematical model of hollow fiber dialyzer is presented. The concentration profile of the inside hollow fiber stream is function of two dimensions of the flow system. The concentration of the dialyzate is function of axial direction of the dialyzer only. In the end, the solution is examined by evaluating different system parameter.
CHAPTER TWO

REVIEW OF LITERATURE

Concept and Description of A Hollow Fiber Dialyzer Unit

The concept of dialysis is based on the semi-permeable membrane. In contrast, water and species of low and medium molecular weight can freely permeate the membranes, which allow the solutes in the stream to pass through the membrane into the dialyzing fluid, until an equilibrium is achieved between the stream and the dialyzate.

It is assume that the group of molecules whose dimensions are relatively small are permitted to pass from the blood stream through the membrane into the dialyzate fluid. As a result of this, there is a net movement of waste product solutes from a region of higher concentration to a region of lower concentration (dialyzate).

The rate of transfer is governed by the concentration difference across the membrane, the molecular size and the permeability characteristics of the membrane.

The hollow fiber dialyzer system consists of a shell which houses the hollow fiber boundle. The fiber are grouped together in a parallel array with one end sealed and the other open (exposed to atmospheric pressure). Both ends terminate in tube sheet.
length to diameter ratio of a typical channel in a well-packed hollow fiber dialyzer often has a value as large as $10^3$ to $10^4$.

The entry region effect, which is important in ordinary heat exchangers, becomes practically negligible for this kind of unit, which is at the range of $10^2$ - $10^4$ tubes. The Reynolds number for a well-packed hollow fiber dialyzer is very low, that is, the dialysis is carried out with laminar flow. The typical hollow fibers dialysis unit is shown as Figure 1 below:

![Figure 1. Hollow Fiber Dialyzer Unit Scheme](image)

A: Jacket  B: Hollow fibers  
C: Stream inlet  D: Stream outlet  
E: Dialyzate inlet  F: Dialyzate outlet
Review Studies of The Hollow Fiber Dialyzer

To date, very little work on hollow fiber has been reported in the literature.

In 1973, Gill and Bansal introduced the design and analysis of hollow fiber reverse systems. A predicted model is developed using the equivalent annulus assumption. The effects of pressure, temperature, flow rate, concentration, viscosity of the feed, system length, membrane rejection parameter, and number of fibers are studied.

Dandavati and Gill (1975) introduced the experimental work of hollow fiber reverse osmosis. The performance of a hollow fiber reverse osmosis system was determined by measuring the fraction of feed recovered as product, and the concentration reduction ratio.

Noda and Gryte (1979) introduced a mass transfer theoretical investigation of hollow fibers in countercurrent dialysis. In which, mass transfer coefficient are obtained as a function of fiber packing density, membrane thickness, membrane material and solute type.

Papenfuse and Thorson (1979) presented a theoretical investigation of ultrafiltration through hollow fibers used in artificial kidney applications.
CHAPTER THREE

Derivation of Mathematical Model

Mathematical analysis

The mathematical model to be considered in this analysis is illustrated in the Figure 2. below. For simplicity following assumption are made here.

1) Steady state conditions.
2) Laminar flow in stream side provides a fully developed parabolic velocity profile.
3) The diffusion process can be described by Fick's law.
4) Physical properties within the system such as density, diffusivity and overall mass transfer coefficient are constants and independent of concentration.
5) Axial diffusion is insignificant.
6) The dialyzate-side mass transfer resistance is position independent.
7) Plug flow in dialyzate-side.

Figure 2. Flow model of hollow fiber dialyzer.
By referring to Figure 2. and the assumptions above governing equations for a counterflow situation can be formalized for two sub-systems. One for stream-side and another for dialyzate-side.

Stream-side:

\[ V_z \frac{\partial C_A}{\partial Z} = \nabla \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C_A}{\partial r} \right) \]  \tag{1}

with boundary conditions:

1. B.C. 1. at \( Z=0 \), \( C_A = C_{A0} \) at all \( r \)
2. B.C. 2. at \( r=0 \), \( C_A \) finite or \( \frac{\partial C_A}{\partial r} = 0 \)
3. B.C. 3. at \( r=R \), \( -\nabla \frac{\partial C_A}{\partial r} \bigg|_{r=R} = K(C_A|_{r=R} - C_D) \)

where \( C_D \) is the concentration of species A in the dialyzate stream.

Based on the assumption (2), we can substitute

\[ V = V_{max} \left[ 1 - \frac{r^2}{R^2} \right] \]

to equation (1), which becomes

\[ V_{max} \left[ 1 - \frac{r^2}{R^2} \right] \frac{\partial C_A}{\partial Z} = \nabla \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C_A}{\partial r} \right) \]  \tag{2}

Dialyzate-side:

\[ Q_D \frac{dC_D}{dZ} = -2\pi RN \cdot K(C_A|_{r=R} - C_D) \]  \tag{3}

with boundary condition

4. B.C. 4. at \( Z=L \), \( C_D = C_{DL} \)

Total mass balance of A between two streams

\[ Q_D (C_{DO} - C_{DL}) = \frac{N \pi R^2 V_{max}}{2} \left[ C_{A0} - \frac{4}{R^2} \left| C_A \right|_{r=0} \right] + \frac{\pi R^2}{2} \int_{r=0}^{r=R} C_A \left( 1 - \frac{y^2}{R^2} \right) y \, dy \]  \tag{4}
Here: N: number of capillary tubes

\( CA \): \( f(z,r) \) : local solute concentration in the stream

\( CA_0 \): inlet solute concentration of stream

\( CD \): \( f(z) \) : solute concentration in the dialyzate stream

\( CD_L \): inlet solute concentration in the dialyzate stream

\( CD_O \): outlet solute concentration in the dialyzate stream

\( \phi \): binary mass diffusivity

\( K \): the overall mass transfer coefficient

\( Q_D \): volumetric flow rate of the dialyzate stream

\( R \): radius of capillary tubes

\( V_Z \): the velocity in the axial direction

\( V_{max} \): the maximum axial velocity at \( r = 0 \)

---

**Dimensionless Forms of the Model**

Introducing the following dimensionless variables,

\[
\Theta = \frac{CA - CD_L}{CA_0 - CD_L}
\]

\[
\Theta_d = \frac{CA_0 - CD}{CA_0 - CD_L}
\]

\[
\varepsilon = \frac{\gamma}{R}
\]

\[
\beta = \frac{\Theta Z}{V_{max} R^2}
\]

therefore equation (2) can be written as

\[
(1-\varepsilon^2) \frac{\partial \Theta}{\partial \beta} = \frac{1}{\varepsilon} \frac{\partial}{\partial \varepsilon} \left( \varepsilon \frac{\partial \Theta}{\partial \varepsilon} \right)
\]
with boundary conditions:

(1) B.C. 1'. at $\theta = 0$, $\theta = 1$ at all

(2) B.C. 2'. at $\varepsilon = 0$, $\theta = \text{finite or } \frac{\partial \theta}{\partial \varepsilon} = 0$ at all

(3) B.C. 3'. at $\varepsilon = 1$, $\frac{\partial \theta}{\partial \varepsilon} \big|_{\varepsilon=1} = N_{sh} (\theta \big|_{\varepsilon=1} + \theta_d - 1)$

and equation (3) can be formulated as

\[
\frac{d \theta_d}{d \phi} = 2 \cdot \frac{R K}{\phi} \cdot \frac{N \pi R^2 V_{max}}{Q_d} (\theta \big|_{\varepsilon=1} + \theta_d - 1)
\]

\[
\frac{d \theta_d}{d \phi} = 4 \cdot N_{sh} \cdot R_1 (\theta \big|_{\varepsilon=1} + \theta_d - 1)
\]  \hspace{1cm} (7)

with boundary condition

(4) B.C. 4'. at $\phi = \frac{1}{P_e \cdot \frac{1}{R_3^2}}$, $\theta_d = 1$

Here:

$N_{sh} = \frac{R K}{\phi}$ : sherwood number

$P_e = \frac{V_{max} L}{\phi}$ : the length Peclet number

$R_1 = \frac{N \pi R^2 V_{max}}{2 Q_d}$ : volumetric flow rate of stream

\[ \text{volumetric flow rate of dialyzate} \]

$R_3 = \frac{R}{L}$ : the ratio of dimensions of the flow system
Solution by Separation and Transformation of Variables

We can solve equation (6) with boundary conditions. By the method of separation of variables, we let

$$\Theta (\eta, \varepsilon) = Z(\eta) R(\varepsilon)$$

Equation (6) may be decomposed to the following two ordinary differential equations,

$$\frac{1}{Z} \frac{dZ}{d\eta} = -\beta^2$$  \hspace{1cm} (8)

$$\varepsilon \frac{d^2R}{d\varepsilon^2} + \frac{dR}{d\varepsilon} + \varepsilon (1 - \varepsilon^2) \beta^2 R = 0$$  \hspace{1cm} (9)

There are three cases to be considered:

1. when $\beta^2 < 0$,
   It is not valid for the system.

2. when $\beta^2 = 0$,
   $$Z(\eta) = C_01$$  \hspace{1cm} (10)
   $$R(\varepsilon) = C_02 \varepsilon + C_03$$  \hspace{1cm} (11)
   where $C_01$, $C_02$, $C_03$ are arbitrary constant

3. when $\beta^2 > 0$,
   $$\frac{dZ}{d\eta} + \beta^2 Z = 0$$  \hspace{1cm} (12)

   $$\varepsilon \frac{d^2R}{d\varepsilon^2} + \frac{dR}{d\varepsilon} + \varepsilon (1 - \varepsilon^2) \beta^2 R = 0$$  \hspace{1cm} (13)
To solve the ordinary differential equation of the equation (12), we can obtain

\[ Z(p) = C_1 e^{\beta p} \]  \hspace{1cm} (14)

where \( C_1 \) is arbitrary constant.

To solve the second order differential equation of equation (13), the following transformation of both dependent and independent variable are performed:

(I) Let \( U = \beta \varepsilon^2 \)

then

\[ du = 2\beta \varepsilon d\varepsilon \]

\[ \frac{dR}{d\varepsilon} = \frac{dR}{du} \cdot \frac{du}{d\varepsilon} = 2\beta \varepsilon \frac{dR}{du} \]

\[ \frac{d^3R}{d\varepsilon^3} = \frac{d}{d\varepsilon} \left( \frac{dR}{d\varepsilon} \right) = \frac{d}{d\varepsilon} \left( 2\beta \varepsilon \frac{dR}{du} \right) \]

\[ = 2\beta \frac{dR}{du} + 2\beta \varepsilon \frac{d}{du} \frac{du}{d\varepsilon} \frac{dR}{du} \]

\[ = 2\beta \frac{dR}{du} + 4\beta^2 \varepsilon^2 \frac{d^2R}{du^2} \]

Therefore equation (13) becomes

\[ 4\beta^3 \varepsilon^3 \frac{d^2R}{du^2} + 4\beta \varepsilon \frac{dR}{du} + \varepsilon (1-\varepsilon^2) \beta^2 R = 0 \]

\[ U \frac{dR}{du} + \frac{dR}{du} + \frac{B(1-\varepsilon^2)}{4} R = 0 \]  \hspace{1cm} (15)
Let \( R(u) = e^{-u^{1/2}} \cdot S(u) \)

Then
\[
\frac{dR}{du} = -\frac{1}{2} e^{-u^{1/2}} + e^{-u^{1/2}} \frac{dS}{du}
\]

\[
\frac{d^2R}{du^2} = \frac{d}{du} \left( \frac{dR}{du} \right) = \frac{d}{du} \left( -\frac{1}{2} e^{-u^{1/2}} \cdot S + e^{-u^{1/2}} \frac{dS}{du} \right)
\]

\[
= \frac{1}{4} e^{-u^{1/2}} \cdot S - \frac{1}{2} e^{-u^{1/2}} \frac{dS}{du} \cdot \frac{1}{2} e^{-u^{1/2}} \frac{dS}{du} + e^{-u^{1/2}} \frac{d^2S}{du^2}
\]

Then equation (15) becomes
\[
U \frac{d^3S}{du^2} + (1-U) \frac{dS}{du} + \left( \frac{U}{4} + \frac{1}{2} + \frac{B}{4} - \frac{U}{4} \right) S = 0
\]

\[
U \frac{d^2S}{du^2} + (1-U) \frac{dS}{du} - \left( \frac{1}{2} - \frac{B}{4} \right) S = 0 \tag{16}
\]

Equation (16) is in the form of confluent hypergeometric function known as Kummer's equation (Slater, 1960). The standard form of the Kummer's equation and its solution are given in Appendix A. For the case as equation (16) with \( a = 1/2 - \theta/4 \) and \( b = 1 \), the solution are

\[
S_1 = \mathbf{F}_1\left( \frac{1}{2} - \frac{B}{4}; 1; U \right)
\]

\[
S_2 = \mathbf{F}_1\left( \frac{1}{2} - \frac{B}{4}; 1; U \right) \ln U + \sum_{k=1}^{\infty} B_k U^k
\]
Reverse the two solutions of $S_1$ and $S_2$ above by using the transformation of $U$ and $R(u)$ which were previously used before that is

$$R(u) = e^{\frac{U}{2}} \cdot S(u)$$

and

$$U = \beta \varepsilon^2$$

As the result, the following two solutions of in equation (13) can be obtained

$$R_1(\varepsilon) = e^{\beta \varepsilon^2} \varepsilon \cdot F_1(\frac{1}{2} - \frac{\beta}{4} ; l ; \beta \varepsilon^2)$$

(17)

$$R_2(\varepsilon) = e^{\beta \varepsilon^2} [F_1(\frac{1}{2} - \frac{\beta}{4} ; 1 ; \beta \varepsilon^2) \ln(\beta \varepsilon^2) + \sum_{k=1}^{\infty} B_k(\beta \varepsilon^2)^k]$$

(18)

Since equation (17) and (18) are the solutions of equation (13), we can obtain

$$R(\varepsilon) = C_2 e^{\beta \varepsilon^2} F_1(\frac{1}{2} - \frac{\beta}{4} ; l ; \beta \varepsilon^2)$$

$$+ C_3 e^{\beta \varepsilon^2} [F_1(\frac{1}{2} - \frac{\beta}{4} ; 1 ; \beta \varepsilon^2) \ln(\beta \varepsilon^2) + \sum_{k=1}^{\infty} B_k(\beta \varepsilon^2)^k]$$

(19)

where $C_2$, $C_3$ are arbitrary constant.

Since

$$\Theta(\varepsilon, \varphi) = \sum(\varphi) R(\varepsilon)$$

we combine the solutions of the cases discussed before, then

$$\Theta(\varepsilon, \varphi) = C_{01}(C_{02} \varepsilon + C_{03}) + C_1 e^{\beta \varphi} [C_2 e^{\beta \varepsilon^2} F_1(\frac{1}{2} - \frac{\beta}{4} ; l ; \beta \varepsilon^2)$$

$$+ C_3 e^{\beta \varepsilon^2} [F_1(\frac{1}{2} - \frac{\beta}{4} ; 1 ; \beta \varepsilon^2) \ln(\beta \varepsilon^2) + \sum_{k=1}^{\infty} B_k(\beta \varepsilon^2)^k]]$$

(20)

In order for the solution of equation (13) satisfies the boundary condition B.C. 2', namely at $\varepsilon = 0$, $\Theta =$ finite, or $\frac{\partial \Theta}{\partial \varepsilon} = 0$, $C_{02}$ and $C_3$ have to be zero. So equation (20) becomes

$$\Theta(\varepsilon, \varphi) = C_6 + C_4 e^{\beta \varphi} e^{\beta \varepsilon^2} F_1(\frac{1}{2} - \frac{\beta}{4} ; l ; \beta \varepsilon^2)$$

(21)
where $C_6$ is a arbitrary constant.

Since the other two boundary condition cannot be used to solve equation (21) right away, so we solve equation (7) first.

Let $H = 4N_{\text{Sh}}R_1$

then equation (7) becomes

$$\frac{d\theta_d}{dp} - H \theta_d = H (\theta|_{\varepsilon=1} - 1)$$  \hspace{1cm} (22)

where $\theta_d, \theta|_{\varepsilon=1}$ are function of $p$ only, so equation (22) is a typical first order linearly ordinary differential equation, and its solution are given as below.

The solution of equation (22) is

$$\theta_d e^{-Hp} = (1-C_6) e^{-Hp} + C_5$$

$$+ \frac{-H}{\beta^2 + H} C_4 e^{-\beta p/2} e^{-\left(\frac{\beta + H}{R_1}\right)} f\left(\frac{1}{2} - \frac{p}{4}; 1; \beta\right)$$  \hspace{1cm} (23)

where $C_5$ is a arbitrary constant.

Equation (23) must satisfy B.C. 4', i.e., at $p = \frac{1}{P_e} \frac{R_1}{R_3}$, $\theta_d = 1$.

so

$$C_5 = C_6 e^{-\frac{H}{P_e R_3}} + \frac{H}{\beta^2 + H} C_4 e^{-\beta p/2} \frac{H}{P_e R_3} f\left(\frac{1}{2} - \frac{p}{4}; 1; \beta\right)$$

Then substitute $C_5$ into equation (23), we can obtain

$$\theta_d(p) = C_6 \left[ e^{-\frac{H}{P_e R_3}} - 1 \right] + 1$$

$$+ \frac{H}{\beta^2 + H} C_4 e^{-\beta p/2} f\left(\frac{1}{2} - \frac{p}{4}; 1; \beta\right) \left[ e^{-\left(\frac{H}{P_e R_3} + H\right)} - e^{-\beta p} \right]$$  \hspace{1cm} (24)

Then we combine it with equation (21), use boundary condition B.C. 3', namely at $\varepsilon = 1$, $-\frac{\partial \theta}{\partial \varepsilon}|_{\varepsilon=1} = N_{\text{Sh}} (\theta|_{\varepsilon=1} + \theta_d - 1)$.
we can find $C_6$ has to be zero, and
\[
\left[ \beta_n e^{-\beta_n \bar{z}_1} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \right) - 2 \beta_n e^{-\beta_n \bar{z}_2} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 2; \beta_n \right) \right]
= N_{sh} e^{-\beta_n \bar{z}_1} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \right) \left[ 1 + \frac{H}{\beta_n + H} \left( e^{\beta_n \bar{z}_1} - 1 \right) \right] \] (25)

Since boundary condition B.C. 3' is satisfied for all $f$, then equation (25) becomes
\[
\left[ \beta_n e^{-\beta_n \bar{z}_1} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \right) - 2 \beta_n e^{-\beta_n \bar{z}_2} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 2; \beta_n \right) \right] \frac{1}{Pe R_e^3}
= N_{sh} e^{-\beta_n \bar{z}_1} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \right) \left[ \frac{\beta_n^2}{\beta_n^2 + H} \frac{1}{Pe R_e^3} + \frac{H}{\beta_n \left( \beta_n^2 + H \right)} \left( 1 - e^{-\frac{(\beta_n^2 + H)}{Pe R_e^3}} \right) \right] \] (26)

The eigenvalues $\beta_n$ can be evaluated from equation (26). The secant method was employed to compute the eigenvalues via UNIVAC Computer. The computer program is given in Appendix C.

After we solve for eigenvalues, the equation (21) becomes
\[
\Theta (\epsilon, \eta) = \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n \epsilon^2 / 2} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \epsilon^3 \right) \] (27)
which must satisfy boundary condition B.C. 1' $\eta = 0$, $\Theta = 1$ that is
\[ 1 = \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n \epsilon^2 / 2} f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \epsilon^3 \right) \] (28)

An equation of the form of equation (9) with the boundary conditions constitutes a Strum-Liouville system (Mickley et al., 1957). The coefficients of solution, $C_{4n}$, may be obtained by making use of the orthogonal properties of the eigenfunctions. Which shown in Appendix B.

\[
C_{4n} = \frac{\frac{1}{\beta_n} e^{-\beta_n \bar{z}_1} \left[ f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \right) - (1 - \frac{\beta_n}{\beta_n^3}) f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 2; \beta_n \right) \right]}{\int_{\epsilon = 0}^{\epsilon = 1} \left( \epsilon - \epsilon^3 \right) e^{-\beta_n \epsilon^2 / 2} \left[ f_1 \left( \frac{1}{2} - \frac{\beta_n}{\beta_n^3}; 1; \beta_n \epsilon^3 \right) \right]^2 d\epsilon} \] (29)
The integrals in the denominator of equation (29) can be evaluated by numerical integration. The Newton-Coates Trapezoidal rule combined with Romberg extrapolation technique was employed to hasten the convergence (Carnahan, 1969). The numerical value of the first thirty $\beta_n$ and $C_{4n}$ are tabulated in Table 1.

The final solution of dialyzate stream concentration becomes

$$\Theta_d(p) = \frac{H}{\beta_n^2 + H} \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n^2} F_i \left( \frac{1}{2} - \frac{\beta_n}{Z}; 1; \beta_n \right) \left[ e^{-\frac{\left(\beta_n^2 + H\right)}{PeRe^2}} - e^{-\beta_n^2} \right] + 1$$

(30)

Calculation of stream outlet dimensionless bulk concentration

From equation (4), the total mass balance of A between two stream is

$$Q_D(C_{DO} - C_{DL}) = \frac{N\Pi R^2 V_{\text{max}}}{2} \left[ C_{AO} - B \right]$$

(31)

Where B is the bulk concentration of A at the stream outlet.

and

$$B = \frac{2\Pi \int_{y=0}^{y=R} C_A \frac{r}{z} \sqrt{z} \, dz \, dy}{2\Pi \int_{y=0}^{y=R} \sqrt{z} \, dy \, dy}$$

Also from equation (5) we know

$$C_{DO} = C_{AO} - (C_{AO} - C_{DL}) \Theta_d \bigg|_{p=0}$$

$$\therefore C_{DO} = C_{AO} - (C_{AO} - C_{DL}) \left[ \frac{H}{\beta_n^2 + H} \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n^2} F_i \left( \frac{1}{2} - \frac{\beta_n}{Z}; 1; \beta_n \right) \left( e^{-\frac{\left(\beta_n^2 + H\right)}{PeRe^2}} - 1 \right) \right] + 1$$

(32)
Substitute equation (32) into equation (31), then rearrange we can obtain

\[ \frac{B}{C_{A_0}} = 1 + \frac{1}{R_1} \left[ \frac{H}{R_0 + H} \sum_{n=1}^{\infty} \frac{C_{A_n} e^{-\beta_n/2}}{n!} \left( \frac{e^{\beta_n}}{1 - \frac{\beta_n}{4}} \right) \left( e^{\frac{-\beta_n}{Pe^{\beta_n}} - 1} \right) \right] \tag{33} \]

In conclusion, the outgoing bulk concentration of the stream can be calculated from equation (33). The computer program for this problem is given in Appendix C.
TABLE 1

at $R_1 = 1.0$, $P_e = 5 \times 10^6$, $R_3 = 1.33 \times 10^{-4}$, $Nsh = 0.4$

<table>
<thead>
<tr>
<th>BETA (x)</th>
<th>BETA (x)</th>
<th>CN (x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.55731</td>
<td>1.00280</td>
</tr>
<tr>
<td>2</td>
<td>5.24396</td>
<td>-0.13455</td>
</tr>
<tr>
<td>3</td>
<td>9.27607</td>
<td>0.06419</td>
</tr>
<tr>
<td>4</td>
<td>13.28912</td>
<td>-0.03985</td>
</tr>
<tr>
<td>5</td>
<td>17.29657</td>
<td>0.02804</td>
</tr>
<tr>
<td>6</td>
<td>21.30147</td>
<td>-0.02123</td>
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<tr>
<td>7</td>
<td>25.30502</td>
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<tr>
<td>8</td>
<td>29.30772</td>
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</tr>
<tr>
<td>9</td>
<td>33.30983</td>
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<tr>
<td>10</td>
<td>37.31159</td>
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<tr>
<td>11</td>
<td>41.31303</td>
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<tr>
<td>12</td>
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<tr>
<td>14</td>
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<tr>
<td>15</td>
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<tr>
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<tr>
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<tr>
<td>20</td>
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<tr>
<td>21</td>
<td>81.32046</td>
<td>0.00354</td>
</tr>
<tr>
<td>22</td>
<td>85.32086</td>
<td>-0.00332</td>
</tr>
<tr>
<td>BETA (23)</td>
<td>CN (23)</td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>---------</td>
<td></td>
</tr>
<tr>
<td>89.32124</td>
<td>0.00312</td>
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<td>93.32163</td>
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<td>97.32196</td>
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<td></td>
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<tr>
<td>101.32222</td>
<td>-0.00264</td>
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<td>BETA (27)</td>
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</tr>
<tr>
<td>105.32250</td>
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<td>BETA (28)</td>
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<td>-0.00238</td>
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<td>BETA (29)</td>
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<td>0.00227</td>
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<td>BETA (30)</td>
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<td></td>
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<tr>
<td>117.32325</td>
<td>-0.00217</td>
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Figure 3. Dimensionless bulk concentration vs. The ratio of the dimensions of the flow system (Peclet number varies, $R_1=1.0$, $N_{sh}=1.6$)
Figure 4. Dimensionless bulk concentration vs. The ratio of the dimensions of the flow system (Sherwood number varies, R1=1.0, Pe = 5 x 10^6)
CHAPTER FOUR

DISCUSSION

The results of this analytical solution have been examined by adjusting different system parameters, such as Sherwood number, Peclet number and the ratio of dimensions of the flow system.

In Figure 3, the dimensionless bulk concentration of the stream outlet, $B/CA_0$, is plotted as a function of the ratio of dimensions of the flow system, $L/R$, at different Peclet number. It shows that the outlet bulk concentration decreases when the ratio of the dimensions of the flow system increases, but the bulk concentration increases when the Peclet number increases. It means that at higher Peclet number the efficiency of the system is lower. On the other hand, when the $L/R$ ratio is higher (or the length of hollow fiber tube is bigger) then the efficiency is relatively higher. From this figure we can easily determine the Peclet number for a given efficiency at a certain hollow fiber length. For example, if we want to control the outlet efficiency larger than 0.85 at $L/R=2000$, then we have to control the Peclet number less than $1 \times 10^6$ when $R_1=1.0$ and $N_{sh}=1.6$.

In Figure 4, the dimensionless bulk concentration of the stream outlet, $B/CA_0$, is plotted as a function of the
ratio of dimensions of the flow system, $L/R$, at different Sherwood number. It shows that the outlet bulk concentration decreases when the Sherwood number increases for a given length of fiber. That is, at higher Sherwood number the efficiency of the system is higher. For example, if we would like to have the efficiency larger than 0.70 at $L/R=4000$, then we have to control the Sherwood number at larger than 0.4 when $R1=1.0$ and $Pe=5 \times 10^6$.

This mathematical model can be used to predict the concentration profile of the solution and dialyzate in a hollow fiber dialyzer flow system.

For different diffusivity of the stream solution, we have to decide what kind of material should be used for the fiber, what is the most optimal length of the fiber, and how many fibers are needed to achieve the highest efficiency. To solve this kind of problem we can simply use this mathematical model and optimization techniques to design the hollow fiber dialyzer flow system. The Sherwood number, Peclet number and the ratio of the dimensions of the flow system will be the controlling parameters in the design. Once the best range of these parameters are found, a most economical and efficient hollow fiber dialyzer can be designed for dialysis operation.
CONCLUSION

A mathematical model describing the flow characteristics and mass transfer has been developed for the hollow fiber dialyzer in countercurrent dialysis.

The theoretical expressions are developed from a typical Graetz problem for the stream side, and a first order differential equation for the dialyzate side. The solution of the dimensionless concentration profile is obtained as a summation of orthogonal eigenfunctions in closed form, which are given as product of an exponential function and a confluent hypergeometric function.

The analytical solution of the model has been examined by adjusting system parameters, like Sherwood number, Peclet number and the geometry of the system. As expected, at higher Sherwood number and higher L/R ratio the bulk concentration in the stream outlet increases, whereas at higher Peclet number the bulk concentration in the stream outlet decreases. This can be used to optimize dialyzer performance.
REFERENCES


TABLE OF NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>B</td>
<td>bulk concentration of outlet product</td>
</tr>
<tr>
<td>CA</td>
<td>( f_1(r,z) ) : local stream concentration</td>
</tr>
<tr>
<td>CD</td>
<td>( f_2(z) ) : dialyzate concentration</td>
</tr>
<tr>
<td>VZ</td>
<td>local velocity in the inside stream</td>
</tr>
<tr>
<td>( V_{\text{max}} )</td>
<td>maximum velocity of the stream</td>
</tr>
<tr>
<td>D</td>
<td>diffusivity</td>
</tr>
<tr>
<td>K</td>
<td>mass transfer coefficient</td>
</tr>
<tr>
<td>R</td>
<td>Radius of hollow fiber</td>
</tr>
<tr>
<td>QD</td>
<td>dialyzate flow rate</td>
</tr>
<tr>
<td>L</td>
<td>length of hollow fiber</td>
</tr>
<tr>
<td>C_{DL}</td>
<td>inlet solute concentration in dialyzate stream</td>
</tr>
<tr>
<td>CAO</td>
<td>inlet solute concentration of the stream</td>
</tr>
<tr>
<td>N</td>
<td>number of hollow fibers</td>
</tr>
<tr>
<td>C_{DO}</td>
<td>outlet solute concentration of dialyzate stream</td>
</tr>
<tr>
<td>( R_1 )</td>
<td>dimensionless ratio of volumetric flow rate of both stream</td>
</tr>
<tr>
<td>( R_3 )</td>
<td>dimensionless ratio of Radius and length of hollow fibers</td>
</tr>
<tr>
<td>Pe</td>
<td>the length peclet number defined below equation (7)</td>
</tr>
<tr>
<td>N_{sh}</td>
<td>sherwood number defined below equation (7)</td>
</tr>
<tr>
<td>H</td>
<td>dimensionless value defined below equation (22)</td>
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</table>

Greek Letters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>( \Theta )</td>
<td>dimensionless stream concentration</td>
</tr>
<tr>
<td>( \Theta_d )</td>
<td>dimensionless dialyzate concentration</td>
</tr>
</tbody>
</table>
\( \epsilon \) : dimensionless \( r \) direction in Hollow Fibers
\( \phi \) : dimensionless \( z \) direction in dialyzer
\( \beta_n, \beta \) : eigenvalues defined in equation (26)
APPENDIX A

A standard form of the confluent hypergeometric differential equation (Slater, 1960) or the Kummer's equation is

\[ \chi \frac{d^2 Y}{d \chi^2} + (b - \chi) \frac{d Y}{d \chi} - a Y = 0 \quad (A-1) \]

In the case of \( b = 1 \), the two linearly independent solutions are

\[ Y_1 = \frac{e^{-\chi}}{\Gamma(a) \Gamma(b-a) \Gamma(b-a+\chi)} \quad (A-2) \]

and

\[ Y_2 = Y_1 \ln \chi + \sum_{n=1}^{\infty} B_n \chi^n \quad (A-3) \]

where \( \frac{e^{-\chi}}{\Gamma(a) \Gamma(b-a) \Gamma(b-a+\chi)} \) is the general confluent hypergeometric function defined as

\[ \frac{e^{-\chi}}{\Gamma(a) \Gamma(b-a) \Gamma(b-a+\chi)} \quad (A-4) \]

and

\[ B_n = \frac{(a)_n H_n}{(b)_n} \quad (A-5) \]

\[ H_n = \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(a+k)}{(a+\ell)} \quad (A-6) \]

\[ (a)_k = \frac{\Gamma(a+k)}{\Gamma(k)} = a(a+1) \cdots (a+k-1) \quad (A-7) \]

The numerical values of confluent hypergeometric function are tabulated in a book (Slater, 1960). These values may also be calculated from equation (A-4).
A standard form of Sturm-Liouville differential equation is
\[
\frac{d}{dx} \left[ P(x) \frac{dy}{dx} \right] + \left[ Q(x) + \lambda R(x) \right] y = 0 \quad (D-1)
\]
A second order differential equation of the form
\[
Q_0(x) \frac{d^2 y}{dx^2} + Q_1(x) \frac{dy}{dx} + \left[ Q_2(x) + \lambda Q_3(x) \right] y = 0 \quad (D-2)
\]
may be transformed into equation (D-1) by means of the relations
\[
P(x) = \exp\left( \int \frac{Q_1(x)}{Q_0(x)} \, dx \right)
\]
\[
Q(x) = \frac{Q_2(x)}{Q_0(x)} P(x) \quad (D-3)
\]
\[
R(x) = \frac{Q_3(x)}{Q_0(x)} P(x)
\]
from which
\[
\int \left[ \frac{Q(x)}{Q_0(x)} + \lambda R(x) \right] y \, dx = - P(x) \frac{dy}{dx} \bigg|_{x=a}^{x=b} \quad (D-4)
\]
compare equation (9) with (D-1), we can obtain
\[
P(x) = \varepsilon
\]
\[
Q(x) = 0
\]
\[
R(x) = \varepsilon (1 - \varepsilon^2)
\]
so the weighing function for equation (28) is
\[
\varepsilon (1 - \varepsilon^2) e^{-\beta_n \varepsilon^2} F \left( \frac{1}{2} - \frac{\beta_n}{4} ; 1 ; \beta_n \varepsilon^2 \right)
\]
from (D-4), we know

\[ \int_0^1 \varepsilon (1-\varepsilon^2) e^{-\beta_n/2} \mathcal{F}_1 \left( \frac{1}{2} - \frac{\beta_n}{4}; 1; \beta_n \varepsilon^2 \right) d\varepsilon \]

\[ = \frac{1}{\beta_n} \frac{d}{d\varepsilon} \left( e^{-\beta_n/2} \mathcal{F}_1 \left( \frac{1}{2} - \frac{\beta_n}{4}; 1; \beta_n \varepsilon^2 \right) \right) \bigg|_{\varepsilon=1}^{\varepsilon=0} \]

\[ = \frac{1}{\beta_n} e^{-\beta_n/2} \left[ \mathcal{F}_1 \left( \frac{1}{2} - \frac{\beta_n}{4}; 1; \beta_n \right) - (1 - \frac{\beta_n}{2}) \mathcal{F}_1 \left( \frac{3}{2} - \frac{\beta_n}{4}; 2; \beta_n \right) \right] \]

It is the numerator of equation (29).
APPENDIX C

COMMON A REAL(16), BETA(160), GBT(160), GBT(100), EN(100).
*NUM(100)
D6A, B, 30.
D6: 160, I=1:N
CALL HAN(1).
CALL WENDA(I).
CALL DENG(I).
CALL GEN(I).
JENE CONTINUE
CALL OUTPUT(N).
CALL GRT2.
FIN.
FUNCTION F(A,B,Z)
IMPLICIT REAL*8(A-H,O-Z)
LOGICAL FSTTH
D6A, TOL1/1.0D-5/
D=0.06,
F=1.06,
F=1.05,
TERM=1.06,
FSTTH=.TRUE.,
D6 3=30 N=1,560
TERM=TERM+(A*R)*2./PI(B/4))
F=F*T/F
IF (FSTTH, 60 TO 2906)
IF (F .LE. 0.06) GO TO 2906
D=DIJ/2.71OF/F
IF (DIJ .LE. TOL1) RETURN
2906 FSTHR=F
0=0.044,10
P=FR1,10
FSTTH=.TRUE.,
3000 CONTINUE
WRITE (6,706)
6706 FORMAT(/80X,'DEFAULT ON F')
RETURN
END
FUNCTION TEST(X)
IMPLICIT REAL*8(A-H,O-Z)
DATA R395R4, F1, R3/0.4B6,5.0D6,1.0D0,2.22D-3/
A=0.56D0-X/4.10
R=1.10
Z=r
T1=F(A, R, Z)
C=1.50D0-x/4.10
E=2.10
T2=F(C, E, Z)
T3=x
T4=DEXP(-T3/2.10)

- 32 -
BB1=PE*(R3**2.10)
BB=1.10/R3
B3=RNSH
B3=4.10*RNSH**R3
B4=0.5I0-X/4.10
B5=(X**2.10)
B6=R6*10
B7=(B5/R6)*R3
B8=B3-C*2.10
B9=10*X**(-R6*R3)
TEST1=BB**T2**T4**T1I-2.DO*T3*T4*R4*T2*BB1
TEST2=BB**T4**T1*(B7+R8-R8*BB)
TEST=TEST1-TEST2
RETURN
END:

SUBROUTINE RTFNI(I)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/ARTA1/BETA(100),QBET(100),GBET(100),CN(100),
*MINH(100)
DEL: T1=TAI/ST1+STEP /1.0,7.0,110,1.0/ 
X0=ST1+T1
I=1-I
IF (I.GT.1) X0=RTFNI(I)+STEP 
GO TO 500
200 X0=ROOT*X0
500 IF (TEST(X0*TEST(X0+STEP)),LT.0.0) GO TO 1000
X0=X0+STEP
GO TO 500
1000 CONTINUE
CALL RTFNI(ROU,T0,TOL,STEP)
BETA(I)=ROOT
RETURN
END:

SUBROUTINE RTFNI(ROU,T0,TOL,STEP)
IMPLICIT REAL*8(A-H,O-Z)
LOGICAL FSTTIM
FSTTIM=.TRUE.
X1=X0+ST1
I0=1000 I=1,100
X2=(X0*TEST(X1)-X1*TEST(X0))/(TEST(X1)-TEST(X0))
IF (FSTTIM) GO TO 900
IF (BARS(X2-X2STOR).LE.TOL) GO TO 1500
900 IF ((TEST(X2)/TEST(X0),GT.0.0) X0=X2
IF ((TEST(X2)/TEST(X1).GT.0.0) X1=X2
FSTTIM=.FALSE.
X2STOR=X2
1000 CONTINUE
WRITE(6,6833)
6833 FORMAT(*/40X,'DEFUAL ON ROOT')
1500 ROU=X2
RETURN
END

SUBROUTINE WENTA(I)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/ARNH/ BETA(100),QHET(100),GRET(100),CN(100),
*K(I1:100)
BETA=1.0*BETA(1)
BT2=1.0*BETA(1)/2.0
BTF=1.0+BETA(1)/2.0
BT1=0.5+0.5*BETA(1)/4.0
BT1'=BET11:1.0+BETA(1))
BT5=1.5*(BETA(1)/4.0+2.0*BETA(1))
ROOT2=ROOT1**2*BT2*BT5
ROOT3=ROOT1**1.0*BT2**3*BT5
ROOT4=ROOT1**2=ROOT1.3
QHET(I)=ROOT4
RETURN
END

FUNCTION DHT(1,XT)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/ARNH/ BETA(100),QHET(100),GRET(100),CN(100),
*K(I1:100)
F=0.0*(X**2,DO)
F=0.0*(X**4,DO)
A=0.0-BETA(1)/4.0
B=1.0
C=BETA(1)/4.0*(X**2,DO)
D=BETA(1)/4.0+C
E=F*F+G+C
RETURN
END

SUBROUTINE INGRT(G,INTGR,M,FSTPT,ENDPT)
IMPLICIT REAL*8(A-H,O-Z)
DOUBLE PRECISION INTGR
DIMENSION G(10000)
H=1.0/0(D M FLOAT(M))
SUM=FSTPT
M=M-1
DO 2800 K=1,M1
SUM=SUM+H/2.0
CONTINUE 2800
SUM=SUM+ENDPT
INTGR=SUM*H/2.0
RETURN
END

SUBROUTINE ROMBG(KOUNT,T)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION T(15,15)
N=N+1
1600 CONTINUE
RETURN
END
SUBROUTINE BENCA(I)
IMPLICIT REAL*(A-H,O-Z)
LOGICAL FSTIM
DOUBLE PRECISION INT
COMMON/AREA1/ BETA(100), QBET(100), GBET(100), CN(100), NUM(100)
DIMENSION FUNC(10000), T(15,15)
DATA TOL, LIM, I, J, 12/
FSTIM = .FALSE.
FUNC = ONE(T, XI)
T(1,1) = 0.5D0*E14, 0.5D0*ENPT
N = 0
FSTIM = .TRUE.
I0 = 1000, NUM = 2*LIM
H = 1.0D0/(1. FLINT(M:))
XI = 0.1D0*M
M1 = M - 1
DO 2000 J = N+1, M1
FUNC(J) = ONE(T, XI)
XI = XI + 2.0D0*M
2000 CONTINUE
CALL INTGET(FUNC, INT, M, FSTFT, ENPT)
T(KOUNT, 1) = INT
CALL ROMBERG(KOUNT, T)
ROOT1 = T(1,KOUNT)
NUM(I) = H:
IF (FSTIM) GO TO 3000
IF (ABS(ROOT1 - GNSTOR), LE, TOL3) GO TO 17
3000 N = M
M = M/2
GNSTOR = ROOT1
GBET(I) = ROOT1
1000 CONTINUE
RETURN
END
SUBROUTINE CEN(I)
IMPLICIT REAL*(A-H,O-Z)
COMMON/AREA1/ BETA(100), QBET(100), GBET(100), CN(100), NUM(100)
CN(1)=QRET(1)/BETA(1)
RETURN
END
SUBROUTINE OUTPUT(I)
IMPLICIT REAL*8(A-H,0-Z)
COMMON/AREA1/, BETA(100), QRET(100), GBET(100), CN(100),
*SUM(100),
DO 5000 I=1,N
WRITE(6,2000) I, BETA(I), T, GBET(I), I, CN(I)
2000 FORMAT(*4X,6H1BT (,'12.4H) = 'F10.5,4X,6HG2ET ('12.4H)
*F12.5,
*3X,6H4FN (,'12.4H) = 'F8.5,5X,4HCN ('12.4H) = 'E12.5)
5000 CONTINUE
RETURN
END
SUBROUTINE GRATZ
IMPLICIT REAL*8(A-H,0-Z)
COMMON/AREA1/, BETA(100), QRET(100), GBET(100), CN(100),
*NUM(100),
IN=1.0, EPS=1.0, A=1.0
RH=0.40,
PL=5.0, CH=1.0,
R1=1.0, R2=2.22,
R3=2.22,
PH=1.0,
H=4.0, N=5.0
SUM=0.0
DO 1000 I=1,30
RP1=(BETA(I)**2.0)+H
RR2=H/RR1
RP3=EXP(-BETA(I)/2.0)
RR4=6.0*510.-BETA(I)/4.0+1.0*BETA(I))
RR5=RP3**4.0*RR3**2.0)
RR6=RP3**2.0*RR5
RR7=RR6-1.0
BULK=RP3**3.0*CN(1)**3.0**0.0**0.0*RR6/RR1
ASUM=BULK+SUM
TT=ASUM-SUM
T=INPS(TT)
IF (1-.EPS) 3,3,5
5 SUM=ASUM
1000 CONTINUE
THULK=SUM+PF
GO TO 6
3 THULK=ASUM+PF
6 WRITE(6,444) I
444 FORMAT(*5X,'SUMMATION TERMS=','2X,I2)
WRITE(6,555) PE, THULK
555 FORMAT(*5X,'PF=','1X,E14.5,2X,'BULK CONC.=','2X,F12.6)
RETURN
END