MATHEMATICAL MODELING OF MASS TRANSFER IN A HOLLOW FIBER DIALYZER

BY

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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, where as at higher Sherwood number and higher L/R ratio the bulk concentration increases. This can be used to optimize dialyzer performance.

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CHAPTER ONE

INTRODUCTION

Liquid-phase membrane seperation process (such as dialysis, reverse osmosis and ultrafiltration) utilize the difference in the membrane permeability of molecules as a basis for seperation. 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 defferent 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 membrene 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 concentretion (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. the 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 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 :

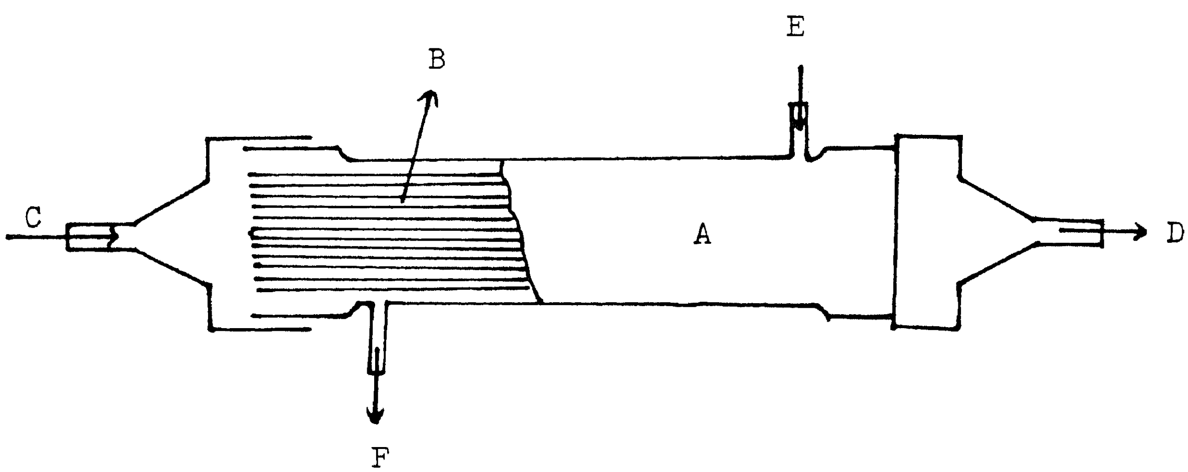

Figure 1. Hollow Fiber Dialyzer Unit Scheme

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 ultrafiltr tion 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 with in the system such as density, diffusivity and overall mass transfer coefficient are contants 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.

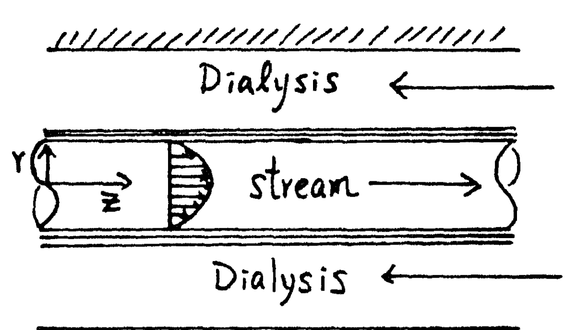

Figure 2. Flow model of hollow fiber dialyzer.

By refering to Figure 2. and the assumptions above govering equations for a counterflow situation can be formalated for two sub-systems. One for stream-side and another for dialyzate-side.

Stream-side:

$$V_z \frac{\partial C_A}{\partial Z} = \mathcal{D} \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial C_A}{\partial r}\right) \qquad (1)$$

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, $-\mathcal{D} \frac{\partial C_A}{\partial r}\Big|_{r=R} = K\left(C_A|_{r=R} - C_D\right)$

where C_D is the concentration of spceies A in the dialyzate stream.

Base on the assumption (2), we can substitute

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

to equation (1), which becomes

$$V_{max}\left[1 - \frac{r^2}{R^2}\right] \frac{\partial C_A}{\partial Z} = \mathcal{D} \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial C_A}{\partial r}\right) \qquad (2)$$

Dialyzate-side:

$$Q_D \frac{dC_D}{dZ} = -2\pi R N \cdot K\left(C_A|_{r=R} - C_D\right) \qquad (3)$$

with boundary condition

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

Total mass balance of A between two stream

$$Q_D\left(C_{D0} - C_{DL}\right) = \frac{N\pi R^2 V_{max}}{2}\left[C_{A0} - \frac{4}{R^2}\int_{r=0}^{r=R} C_A\Big|_{Z=L} \cdot \left(1 - \frac{r^2}{R^2}\right) r\,dr \qquad (4)$$

Here: N: number of capillary tubes

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

C_{AO}: inlet solute concentration of stream

C_D: f(z) : solute concentration in the dialyzate stream

C_{DL}: inlet solute concentration in the dialyzate stream

C_{DO}: outlet solute concentration in the dialyzate stream

: binary mass diffusivity

K : the overall mass transfer coefficient

Q_D : volumetric flow rate of the dialyzate stream

R : fadius 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,

$$\theta = \frac{C_A - C_{DL}}{C_{Ao} - C_{DL}}$$

$$\theta_d = \frac{C_{Ao} - C_D}{C_{Ao} - C_{DL}} \qquad (5)$$

$$\varepsilon = \frac{r}{R}$$

$$\rho = \frac{\mathscr{D} Z}{V_{max} R^2}$$

therefore equation (2) can be written as

$$(1-\varepsilon^2)\frac{\partial \theta}{\partial \rho} = \frac{1}{\varepsilon}\frac{\partial}{\partial \varepsilon}\left(\varepsilon \frac{\partial \theta}{\partial \varepsilon}\right) \qquad (6)$$

with boundary conditions:

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

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

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

and equation (3) can be formulated as

$$\frac{d\theta_d}{d\rho} = 2 \cdot \frac{RK}{\mathscr{D}} \cdot \frac{N\pi R^2 V_{max}}{Q_D}\left(\theta|_{\varepsilon=1} + \theta_d - 1\right)$$

$$\frac{d\theta_d}{d\rho} = 4 \cdot N_{sh} \cdot R_1 \left(\theta|_{\varepsilon=1} + \theta_d - 1\right) \qquad (7)$$

with boundary condition

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

Here:

$N_{sh} = \frac{RK}{\mathscr{D}}$: sherwood mumber

$P_e = V_{max} L/\mathscr{D}$: the length Peclet number

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

$R_3 = \frac{R}{L}$: the ratio of dimensions of the flow system

Solution by Seperation and Transformation of variables

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

$$\theta(\rho, z) = Z(\rho) R(\varepsilon)$$

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

$$\frac{1}{Z}\frac{dZ}{d\rho} = -\beta^2 \qquad (8)$$

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

There are three cases to be considered:

(1) when $\beta^2 < 0$,

It is not valid for the system.

(2) when $\beta^2 = 0$,

$$Z(\rho) = C_{01} \qquad (10)$$

$$R(\varepsilon) = C_{02}\varepsilon + C_{03} \qquad (11)$$

where C_{01}, C_{02}, C_{03} are arbitrary constant

(3) when $\beta^2 > 0$,

$$\frac{dZ}{d\rho} + \beta^2 Z = 0 \qquad (12)$$

$$\varepsilon\frac{d^2R}{d\varepsilon^2} + \frac{dR}{d\varepsilon} + \varepsilon(1-\varepsilon^2)\beta^2 R = 0 \qquad (13)$$

To solve the ordinary differential equation of the equation (12), we can obtain

$$Z(\rho) = C_1 e^{-\beta^2 \rho} \tag{14}$$

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

$$du = 2\beta\varepsilon \, d\varepsilon$$

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

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

$$= 2\beta\frac{dR}{du} + 2\beta\varepsilon\frac{d}{du}\cdot\frac{du}{d\varepsilon}\frac{dR}{du}$$

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

Therefore equation (13) becomes

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

$$u\frac{d^2R}{du^2} + \frac{dR}{du} + \frac{\beta(1-\varepsilon^2)}{4}R = 0 \tag{15}$$

(II) Let $R(u) = e^{-u/2} \cdot S(u)$

Then

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

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

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

Then equation (15) becomes

$$u \frac{d^2S}{du^2} + (1-u)\frac{dS}{du} + \left(\frac{u}{4} + \frac{-1}{2} + \frac{\beta}{4} - \frac{u}{4}\right) S = 0$$

$$u \frac{d^2S}{du^2} + (1-u)\frac{dS}{du} - \left(\frac{1}{2} - \frac{\beta}{4}\right) S = 0 \qquad (16)$$

Equation (16) is in the form of confluent hypergemetric function knows 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 $a = 1/2 - \beta/4$ and $b = 1$, the solution are

$$S_1 = {}_1F_1\left(\frac{1}{2} - \frac{\beta}{4}; 1; u\right)$$

$$S_2 = {}_1F_1\left(\frac{1}{2} - \frac{\beta}{4}; 1; u\right) \ln u + \sum_{k=1}^{\infty} B_k u^k$$

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 $R(u) = e^{-u/2} \cdot S(u)$

and $u = \beta \varepsilon^2$

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

$$R_1(\varepsilon) = e^{-\beta\varepsilon^2/2} \cdot {}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) \tag{17}$$

$$R_2(\varepsilon) = e^{-\beta\varepsilon^2/2}\left[{}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) \ln(\beta\varepsilon^2) + \sum_{k=1}^{\infty} B_k (\beta\varepsilon^2)^k\right] \tag{18}$$

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

$$R(\varepsilon) = C_2\, e^{-\beta\varepsilon^2/2}\, {}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) + C_3\, e^{-\beta\varepsilon^2/2}\left[{}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) \ln(\beta\varepsilon^2) + \sum_{k=1}^{\infty} B_k (\beta\varepsilon^2)^k\right] \tag{19}$$

where C_2 , C_3 are arbitrary constant.

Since $\theta(\varepsilon, \rho) = Z(\rho) R(\varepsilon)$

we combine the solutions of the cases discussed before, then

$$\theta(\varepsilon, \rho) = C_{01}(C_{02}\varepsilon + C_{03}) + C_1 e^{-\beta^2\rho}\left\{C_2 e^{-\beta\varepsilon^2/2}\, {}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) + C_3 e^{-\beta\varepsilon^2/2}\left[{}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) \ln(\beta\varepsilon^2) + \sum_{k=1}^{\infty} B_k (\beta\varepsilon^2)^k\right]\right\} \tag{20}$$

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

$$\theta(\varepsilon, \rho) = C_6 + C_4 e^{-\beta^2\rho} \cdot e^{-\beta\varepsilon^2/2}\, {}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta}{4}; 1; \beta\varepsilon^2\right) \tag{21}$$

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 $H = 4 \cdot N_{sh} R1$

then equation (7) becomes

$$\frac{d\theta_d}{d\rho} - H\theta_d = H\left(\theta|_{\varepsilon=1} - 1\right) \qquad (22)$$

where θ_d, $\theta|_{\varepsilon=1}$ are function of ρ 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

$$\theta_d e^{-H\rho} = (1-C_6)e^{-H\rho} + C_5 + \frac{-H}{\beta^2+H} C_4 e^{-\beta/2} e^{-(\beta^2+H)\rho} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta}{4};1;\beta\right) \qquad (23)$$

where C_5 is a arbitrary constant.

Equation (23) must satisfy B.C. 4'., ie, at $\rho = \frac{1}{Pe}\cdot\frac{1}{R_3^2}$, $\theta_d = 1$

so $$C_5 = C_6 e^{-\frac{H}{PeR_3^2}} + \frac{H}{\beta^2+H} C_4 e^{-\beta/2} e^{\frac{-(\beta^2+H)}{PeR_3^2}} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta}{4};1;\beta\right)$$

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

$$\theta_d(\rho) = C_6\left[e^{\left(\frac{-H}{PeR_3^2}+H\rho\right)} - 1\right] + 1 + \frac{H}{\beta^2+H} C_4 e^{-\beta/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta}{4};1;\beta\right)\left[e^{\left(\frac{-(\beta^2+H)}{PeR_3^2}+H\rho\right)} - e^{-\beta^2\rho}\right] \qquad (24)$$

Then we combine it with equation (21), use boundary condition B.C. 3'.,namely at $\varepsilon = 1$, $-\frac{\partial\theta}{\partial\varepsilon}\Big|_{\varepsilon=1} = N_{sh}\left(\theta|_{\varepsilon=1} + \theta_d - 1\right)$

we can find C_6 has to be zero, and

$$\left[\beta_n e^{-\beta_n/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right)-2\beta_n e^{-\beta_n/2}\left(\tfrac{1}{2}-\tfrac{\beta_n}{4}\right){}_1F_1\left(\tfrac{3}{2}-\tfrac{\beta_n}{4};2;\beta_n\right)\right]$$
$$=N_{sh}\, e^{-\beta_n/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right)\left[1+\frac{H}{\beta_n^2+H}\left(e^{(\beta_n^2+H)(\xi-\frac{1}{PeR_3^2})}-1\right)\right] \qquad (25)$$

Since boundary condition B.C. 3'. is satisfied for all ξ, then equation (25) becomes

$$\left[\beta_n e^{-\beta_n/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right)-2\beta_n e^{-\beta_n/2}\left(\tfrac{1}{2}-\tfrac{\beta_n}{4}\right){}_1F_1\left(\tfrac{3}{2}-\tfrac{\beta_n}{4};2;\beta_n\right)\right]\frac{1}{Pe}\cdot\frac{1}{R_3^2}$$
$$=N_{sh}\, e^{-\beta_n/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right)\left[\frac{\beta_n^2}{\beta_n^2+H}\cdot\frac{1}{Pe}\cdot\frac{1}{R_3^2}+\frac{H}{(\beta_n^2+H)}\left(1-e^{\frac{-(\beta_n^2+H)}{PeR_3^2}}\right)\right] \qquad (26)$$

The eigenvalues β_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

$$\theta(\varepsilon,\xi)=\sum_{n=1}^{\infty} C_{4n}\, e^{-\beta_n\varepsilon^2/2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\varepsilon^2\right)\cdot e^{-\beta_n^2\xi} \qquad (27)$$

which must satisfy boundary condition B.C. 1' $\xi=0,\ \theta=1$

that is

$$1=\sum_{n=1}^{\infty} C_{4n}\, e^{-\beta_n\varepsilon^2} {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\varepsilon^2\right) \qquad (28)$$

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

$$C_{4n}=\frac{\frac{1}{\beta_n}e^{-\beta_n/2}\left[{}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right)-\left(1-\tfrac{\beta_n}{2}\right){}_1F_1\left(\tfrac{3}{2}-\tfrac{\beta_n}{4};2;\beta_n\right)\right]}{\int_{\varepsilon=0}^{\varepsilon=1}(\varepsilon-\varepsilon^3)\, e^{-\beta_n\varepsilon^2}\left[{}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\varepsilon^2\right)\right]^2 d\varepsilon} \qquad (29)$$

The integrals in the denomiantor 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 β_n and C_{4n} are tabulated in Table 1.

The final solution of dialyzate stream concentration becomes

$$\theta_d(\rho) = \frac{H}{\beta_n^2 + H} \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n/2} {}_1F_1\left(\frac{1}{2} - \frac{\beta_n}{4}; 1; \beta_n\right)\left[e^{\left(\frac{-(\beta_n^2+H)}{Pe R_3^2} + H\rho\right)} - e^{-\beta_n^2 \rho}\right] + 1 \tag{30}$$

<u>Calculation of stream outlet dimensionless bulk concentration</u>

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

$$Q_D(C_{D0} - C_{DL}) = \frac{N\pi R^2 V_{max}}{2}\left[C_{A0} - B\right] \tag{31}$$

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

and

$$B = \frac{2\pi \int_{r=0}^{r=R} C_A|_{z=L} V_z r\,dr}{2\pi \int_{r=0}^{r=R} V_z r\,dr}$$

Also from equation (5) we know

$$C_{D0} = C_{A0} - (C_{A0} - C_{DL})\,\theta_d\big|_{\rho=0}$$

$$\therefore C_{D0} = C_{A0} - (C_{A0} - C_{DL})\left[\frac{H}{\beta_n^2 + H} \sum_{n=1}^{\infty} C_{4n} e^{-\beta_n/2} {}_1F_1\left(\frac{1}{2} - \frac{\beta_n}{4}; 1; \beta_n\right)\left(e^{\frac{-(\beta_n^2+H)}{Pe R_3^2}} - 1\right) + 1\right] \tag{32}$$

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

$$\frac{B}{C_{A_0}} = 1 + \frac{1}{R_1}\left[\frac{H}{\beta_n^2+H}\sum_{n=1}^{\infty} C_{4n}\, e^{-\beta_n/2}\, {}_1F_1\left(\frac{1}{2}-\frac{\beta_n}{4};1;\beta_n\right)\left(e^{\frac{-(\beta_n^2+H)}{PeR_3^2}}-1\right)\right] \quad (33)$$

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= 5×10^6 , R_3= 1.33×10^{-4}, **Nsh** =0.4

BETA	(1)	=	0.55731	CN	(1)	=	1.00280
BETA	(2)	=	5.24396	CN	(2)	=	-0.13455
BETA	(3)	=	9.27607	CN	(3)	=	0.06419
BETA	(4)	=	13.28912	CN	(4)	=	-0.03985
BETA	(5)	=	17.29657	CN	(5)	=	0.02804
BETA	(6)	=	21.30147	CN	(6)	=	-0.02123
BETA	(7)	=	25.30502	CN	(7)	=	0.01686
BETA	(8)	=	29.30772	CN	(8)	=	-0.01385
BETA	(9)	=	33.30983	CN	(9)	=	0.01168
BETA	(10)	=	37.31159	CN	(10)	=	-0.01003
BETA	(11)	=	41.31303	CN	(11)	=	0.00875
BETA	(12)	=	45.31426	CN	(12)	=	-0.00773
BETA	(13)	=	49.31532	CN	(13)	=	0.00691
BETA	(14)	=	53.31624	CN	(14)	=	-0.00622
BETA	(15)	=	57.31705	CN	(15)	=	0.00565
BETA	(16)	=	61.31777	CN	(16)	=	-0.00516
BETA	(17)	=	65.31842	CN	(17)	=	0.00474
BETA	(18)	=	69.31900	CN	(18)	=	-0.00438
BETA	(19)	=	73.31953	CN	(19)	=	0.00406
BETA	(20)	=	77.32001	CN	(20)	=	-0.00378
BETA	(21)	=	81.32046	CN	(21)	=	0.00354
BETA	(22)	=	85.32086	CN	(22)	=	-0.00332

BETA	(23)	= 89.32124	CN	(23)	= 0.00312
BETA	(24)	= 93.32163	CN	(24)	= -0.00294
BETA	(25)	= 97.32196	CN	(25)	= 0.00278
BETA	(26)	= 101.32222	CN	(26)	= -0.00264
BETA	(27)	= 105.32250	CN	(27)	= 0.00250
BETA	(28)	= 109.32277	CN	(28)	= -0.00238
BETA	(29)	= 113.32302	CN	(29)	= 0.00227
BETA	(30)	= 117.32325	CN	(30)	= -0.00217

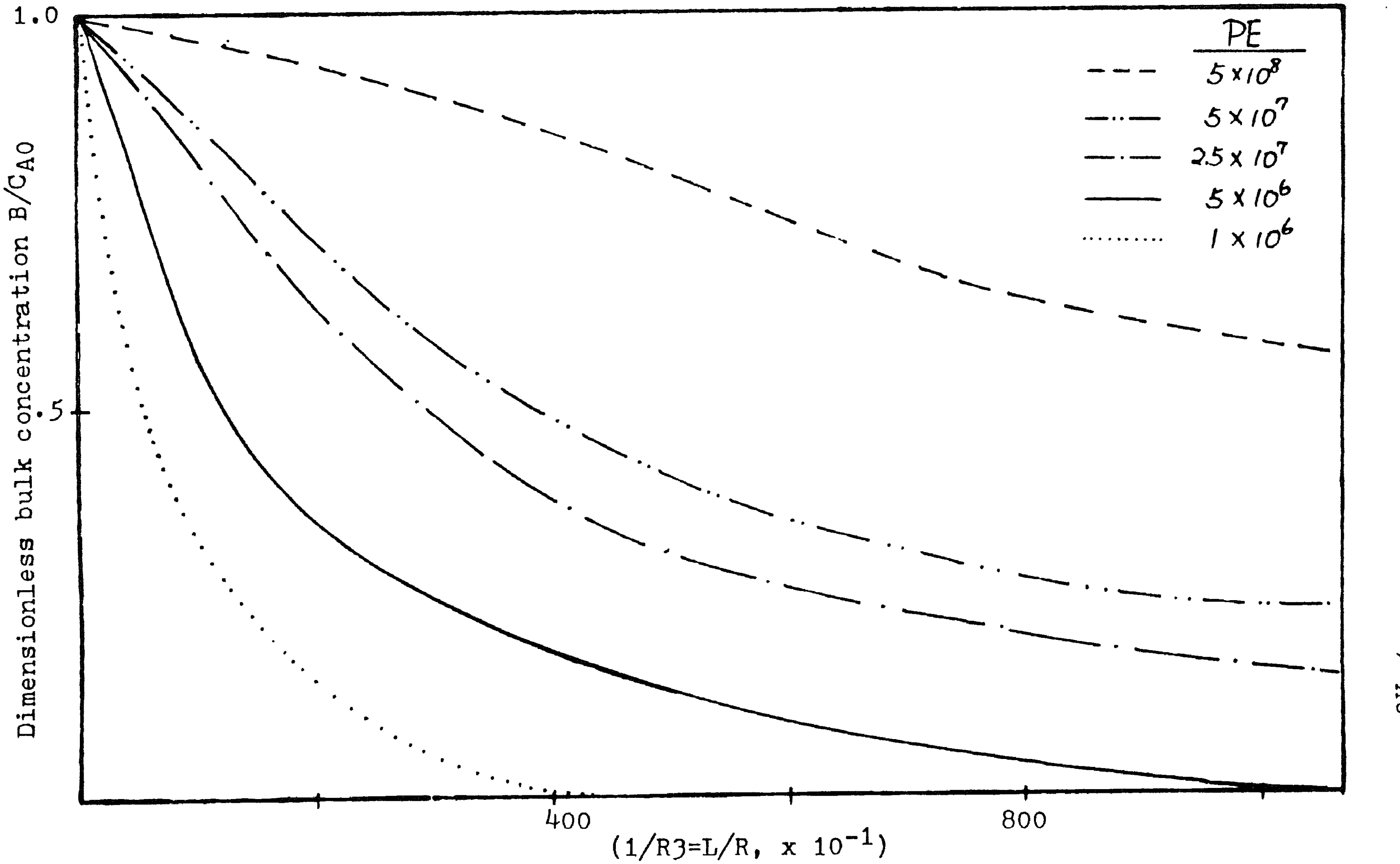

Figure. 3. Dimensionless bulk concentration .vs. The ratio of the dimensions of the flow system (Peclet number varies, R1=1.0, Nsh=1.6)

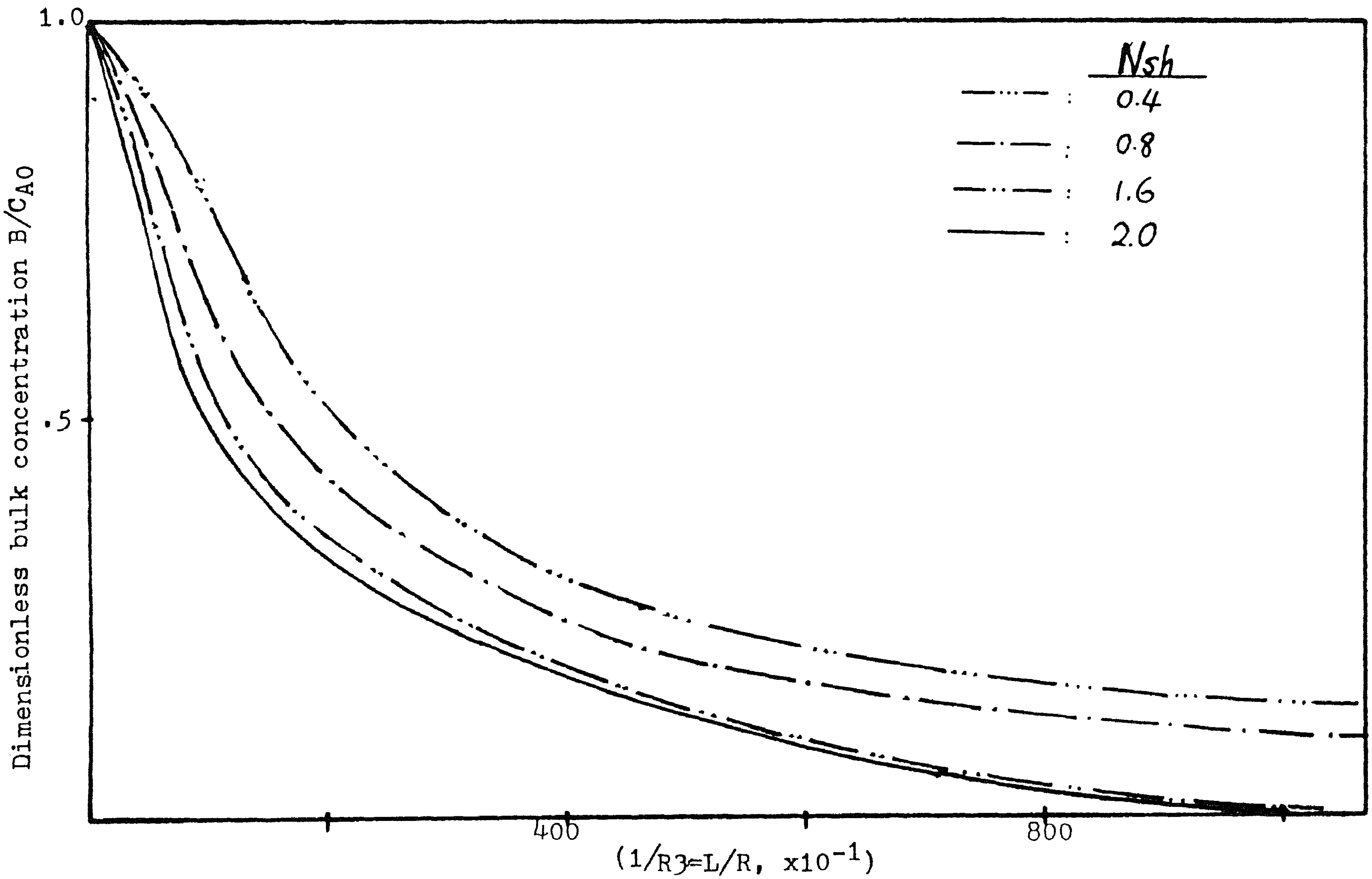

Figure 4. Dimensionless bulk concentration .vs. The ratio of the dimensions of the flow system (Sherwood number varies, R1=1.0, Pe= 5 $\times 10^{6}$)

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/C_{A0} , 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 1×10^6 when R1=1.0 and Nsh=1.6 .

In Figure 4, the dimensionless bulk concentration of the stream outlet, B/C_{A0} , 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 x 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, where as at higher Peclet number the bulk concentration in the stream outlet decreases. This can be used to optimize dialyzer performance.

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TABLE OF NOMENCLATURE

B	:	bulk concentration of outlet product
C_A	:	$f_1(r,z)$: local stream concentration
C_D	:	$f_2(z)$: dialyzate concentration
V_Z	:	local velocity in the inside stream
V_{max}	:	maximum velocity of the stream
D	:	diffusivity
K	:	mass transfer coefficient
R	:	Radius of hollow fiber
Q_D	:	dialyzate flow rate
L	:	length of hollow fiber
C_{DL}	:	inlet solute concentration in dialyzate stream
C_{AO}	:	inlet solute concentration of the stream
N	:	number of hollow fibers
C_{DO}	:	outlet solute concentration of dialyzate stream
R_1	:	dimensionless ratio of volumetric flow rate of both stream
R_3	:	dimensionless ratio of Radius and length of hollow fibers
P_e	:	the length peclet number defined below equation (7)
N_{sh}	:	sherwood number defined below equation (7)
H	:	dimensionless value difined below equation (22)

Greek Letters

θ	:	dimensionless stream concentration
θ_d	:	dimensionless dialyzate concentration

ε : dimensionless r direction in Hollow Fibers

ρ : dimensionless z direction in dialyzer

β_n, β : eigenvalues defined in equation (26)

APPENDIX A

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

$$X\frac{d^2Y}{dX^2} + (b-X)\frac{dY}{dX} - aY = 0 \qquad (A-1)$$

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

$$Y_1 = {}_1F_1(a;1;X) \qquad (A-2)$$

and

$$Y_2 = Y_1 \ln X + \sum_{n=1}^{\infty} B_K X^K \qquad (A-3)$$

where ${}_1F_1(a;b;x)$ is the general confluent hypergeometric function defined as

$${}_1F_1(a;b;X) = \sum_{n=0}^{\infty} \frac{(a)_n X^n}{(b)_n n!} \qquad (A-4)$$

and

$$B_K = \frac{(a)_K H_K}{(K!)^2} \qquad (A-5)$$

$$H_K = \sum_{\ell=0}^{K-1} \left(\frac{1}{a+\ell} - \frac{2}{\ell+1}\right) \qquad (A-6)$$

$$(a)_K = \frac{\Gamma(a+K)}{\Gamma(K)} = a(a+1)\cdots\cdots(a+K-1) \qquad (A-7)$$

The numerical values of confluent hypergeometric function are tabulated in a book (Slater, 1960). These values may also be calculated from equation (A-4).

APPENDIX B

A standard form of Sturm-Liouville differential equation is

$$\frac{d}{dX}\left[P(X)\frac{dY}{dX}\right] + \left[q(X) + \lambda\, r(X)\right] dY = 0 \qquad (D\text{-}1)$$

A second order differential equation of the form

$$g_0(X)\frac{d^2Y}{dX^2} + g_1(X)\frac{dY}{dX} + \left[g_2(X) + \lambda\, g_3(X)\right]Y = 0 \qquad (D\text{-}2)$$

may be transformed into equation (D-1) by means of the relations

$$P(X) = \exp\int \frac{g_1(X)}{g_0(X)}\,dX$$

$$q(X) = \frac{g_2(X)}{g_0(X)}\,P(X) \qquad (D\text{-}3)$$

$$r(X) = \frac{g_3(X)}{g_0(X)}\,P(X)$$

from which

$$\int \left[q(X) + \lambda\, r(X)\right] Y\, dX = -P(X)\frac{dY}{dX}\Bigg|_{X=a}^{X=b} \qquad (D\text{-}4)$$

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

$$\varepsilon(1-\varepsilon^2)\, e^{-\beta_n \varepsilon^2}\, {}_1F_1\left(\tfrac{1}{2} - \tfrac{\beta_n}{4};\, 1;\, \beta_n \varepsilon^2\right)$$

from (D-4), we know

$$\int_0^1 \varepsilon(1-\varepsilon^2)\, e^{-\beta_n/2}\, {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\varepsilon^2\right) d\varepsilon$$

$$= \frac{-\varepsilon}{\beta_n^2}\frac{d}{d\varepsilon}\left(e^{-\beta_n/2\,\varepsilon^2}\, {}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\varepsilon^2\right)\right)\Bigg|_{\varepsilon=0}^{\varepsilon=1}$$

$$= \frac{1}{\beta_n} e^{-\beta_n/2}\left[{}_1F_1\left(\tfrac{1}{2}-\tfrac{\beta_n}{4};1;\beta_n\right) - \left(1-\tfrac{\beta_n}{2}\right){}_1F_1\left(\tfrac{3}{2}-\tfrac{\beta_n}{4};2;\beta_n\right)\right]$$

It is the numerator of equation (29).

APPENDIX C

```
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      DATA N/30/
      DO 1000 I=1,N
      CALL BTAFN(I)
      CALL WENTA(I)
      CALL DENCA(I)
      CALL CEN(I)
 1000 CONTINUE
      CALL OUTPUT(N)
      CALL GRATZ
      STOP
      END
      FUNCTION F(A,B,Z)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL FSTTIM
      DATA TOL1/1.D-5/
      Q=0.D0
      P=1.D0
      F=1.D0
      TERM=1.D0
      FSTTIM=.TRUE.
      DO 3000 N=1,500
      TERM=TERM*(A+Q)*Z/(P*(B+Q))
      F=F+TERM
      IF (FSTTIM) GO TO 2900
      IF(F.EQ.0.D0) GO TO 2900
      DIJJ=(F-FSTOR)/F
      IF (DABS(DIJJ).LE.TOL1) RETURN
 2900 FSTOR=F
      Q=Q+1.D0
      P=P+1.D0
      FSTTIM=.FALSE.
 3000 CONTINUE
      WRITE(6,6700)
 6700 FORMAT(/60X,'DEFAULT ON F')
      RETURN
      END
      FUNCTION TEST(X)
      IMPLICIT REAL*8(A-H,O-Z)
      DATA RNSH,PE,P1,R3/0.4D0,5.0D6,1.0D0,2.22D-3/
      A=0.50D0-X/4.D0
      B=1.D0
      Z=X
      T1=F(A,B,Z)
      C=1.50D0-X/4.D0
      E=2.D0
      T2=F(C,E,Z)
      T3=X
      T4=DEXP(-T3/2.D0)
```

```
      BB1=PE*(R3**2.D0)
      B1=1.D0/BB1
      B2=RNSH
      B3=4.D0*RNSH*B1
      B4=0.5D0-X/4.D0
      B5=(X**2.D0)
      B6=B5+B3
      B7=(B5/B6)*B1
      B8=B3/(B6**2.D0)
      B9=DEXP(-B6*B1)
      TEST1=B1*T3*T4*T1-2.D0*T3*T4*B4*T2*B1
      TEST2=B2*T4*T1*(B7+B8-B8*B9)
      TEST=TEST1-TEST2
      RETURN
      END
      SUBROUTINE BTAFN(I)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      DATA TOL2,START,STEP /1.D-7,0.1D0,1.D0/
      X0=START
      K=I-1
      IF(I.GT.1) X0=BETA(K)+STEP
      GO TO 500
   25 X0=ROOT+STEP
  500 IF((TEST(X0)*TEST(X0+STEP)).LT.0.D0) GO TO 1000
      X0=X0+STEP
      GO TO 500
 1000 CONTINUE
      CALL RTFND(ROOT,X0,TOL2,STEP)
      BETA(I)=ROOT
      RETURN
      END
      SUBROUTINE RTFND(ROOT,X0,TOL,STEP)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL FSTTIM
      FSTTIM=.TRUE.
      X1=X0+STEP
      DO 1000 I=1,100
      X2=(X0*TEST(X1)-X1*TEST(X0))/(TEST(X1)-TEST(X0))
      IF(FSTTIM) GO TO 900
      IF(DABS(X2-X2STOR).LE.TOL) GO TO 1500
  900 IF((TEST(X2)/TEST(X0)).GT.0.D0) X0=X2
      IF((TEST(X2)/TEST(X1)).GT.0.D0) X1=X2
      FSTTIM=.FALSE.
      X2STOR=X2
 1000 CONTINUE
      WRITE(6,6833)
 6833 FORMAT(/40X,'DEFAULT ON ROOT')
 1500 ROOT=X2
```

```
      RETURN
      END
      SUBROUTINE WENTA(I)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      BET1=1.D0/BETA(I)
      BET2=DEXP(-BETA(I)/2.D0)
      BET3=1.D0-BETA(I)/2.D0
      BET=0.5D0-BETA(I)/4.D0
      BET4=F(BET,1.D0,BETA(I))
      BET5=F(1.5D0-BETA(I)/4.D0,2.D0,BETA(I))
      ROOT2=BET1*BET2*BET4
      ROOT3=BET1*BET2*BET3*BET5
      ROOT4=ROOT2-ROOT3
      QBET(I)=ROOT4
      RETURN
      END
      FUNCTION ONE(I,XI)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      FUNA=XI-XI*(XI**2.D0)
      FUNB=DEXP((-BETA(I))*XI**2.D0)
      AA=0.5D0-BETA(I)/4.D0
      BB=1.D0
      CC=BETA(I)*(XI**2.D0)
      FUND=F(AA,BB,CC)
      FUNE=FUND*FUND
      FUN=FUNA*FUNB
      ONE=FUN*FUNE
      RETURN
      END
      SUBROUTINE INTGRT(G,INTGRL,M,FSTPT,ENDPT)
      IMPLICIT REAL*8(A-H,O-Z)
      DOUBLE PRECISION INTGRL
      DIMENSION G(10000)
      H=1.D0/(DFLOAT(M))
      SUM=FSTPT
      M1=M-1
      DO 2800 K=1,M1
      SUM=SUM+2.D0*G(K)
 2800 CONTINUE
      SUM=SUM+ENDPT
      INTGRL=SUM*H/2.D0
      RETURN
      END
      SUBROUTINE ROMBRG(KOUNT,T)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION T(15,15)
```

```
      N=KOUNT-1
      DO 1000 J=2,KOUNT
      A=(4.D0**(J-1))*T(N+1,J-1)
      B=T(N,J-1)
      C=(4.D0**(J-1))-1.D0
      T(N,J)=(A-B)/C
      N=N-1
 1000 CONTINUE
      RETURN
      END
      SUBROUTINE DENCA(I)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL FSTTIM
      DOUBLE PRECISION INT
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      DIMENSION FUNC(10000),T(15,15)
      DATA TOL3,LIM/1.D-7,12/
      FSTPT=ONE(I,0.D0)
      ENDPT=ONE(I,1.D0)
      T(1,1)=0.5D0*FSTPT+0.5D0*ENDPT
      M=2
      N=1
      FSTTIM=.TRUE.
      DO 1000 KOUNT=2,LIM
      H=1.D0/(D FLOAT(M))
      XI=0.D0+H
      M1=M-1
      DO 2000 J=N,M1
      FUNC(J)=ONE(I,XI)
      XI=XI+2.D0*H
 2000 CONTINUE
      CALL INTGRT(FUNC,INT,M,FSTPT,ENDPT)
      T(KOUNT,1)=INT
      CALL ROMBRG(KOUNT,T)
      ROOT1=T(1,KOUNT)
      NUM(I)=M
      IF(FSTTIM) GO TO 3000
      IF(DABS(ROOT1-GNSTOR).LE.TOL3) GO TO 17
 3000 N=M
      M=M*2
      GNSTOR=ROOT1
      GBET(I)=ROOT1
 1000 CONTINUE
   17 RETURN
      END
      SUBROUTINE CEN(I)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
```

```
      CN(I)=QBET(I)/GBET(I)
      RETURN
      END
      SUBROUTINE OUTPUT(N)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      DO 5000 I=1,N
      WRITE(6,2000) I,BETA(I),I,QBET(I),I,GBET(I),I,CN(I)
 2000 FORMAT(/4X,6HBETA (,I2,4H) = ,F10.5,4X,6HQBET (,I2,4H)
     *,F12.5,
     *3X,6HGBET (,I2,4H) = ,F8.5,5X,4HCN (,I2,4H) = ,E12.5)
 5000 CONTINUE
      RETURN
      END
      SUBROUTINE GRATZ
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AREA1/ BETA(100),QBET(100),GBET(100),CN(100),
     *NUM(100)
      DATA EPS/1.D-6/
      RNSH=0.4D0
      PE=5.0D6
      R1=1.0D0
      R3=2.22D-3
      PP=1.D0
      H=4.D0*RNSH*R1
      SUM=0.D0
      DO 1000 I=1,30
      RR1=(BETA(I)**2.D0)+H
      RR2=H/RR1
      RR3=DEXP(-BETA(I)/2.D0)
      RR4=F(0.5D0-BETA(I)/4.D0,1.D0,BETA(I))
      RR5=RR1/(PE*R3*R3)
      RR6=DEXP(-RR5)
      RR6=RR6-1.D0
      BULK=RR2*CN(I)*RR3*RR4*RR6/R1
      ASUM=BULK+SUM
      TT=ASUM-SUM
      T=DABS(TT)
      IF(T-EPS) 3,3,5
5     SUM=ASUM
1000  CONTINUE
      TBULK=SUM+PP
      GO TO 6
3     TBULK=ASUM+PP
6     WRITE(6,444) I
444   FORMAT(/,5X,'SUMMATION TERMS=',2X,I2)
      WRITE(6,555) PE,TBULK
555   FORMAT(/,5X,'PE=',1X,E14.5,2X,'BULK CONC.=',2X,F12.6)
      RETURN
      END
```