Global Journal of Science Frontier Research: F
Mathematics and Decision Sciences
Volume 20 Issue 8 Version 1.0 Year 2020
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Shock Propagation in a Hollow-Fiber Hemodialyzer

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Abstract- Hemodialysis (HD) is one type of procedure for eliminating toxic chemicals and infusing bicarbonate in patients with end-stage renal disease (ESRD). We have developed a comprehensive mathematical model to describe the dynamic exchange process of solutes in a prototype hemodialyzer. The model, which is represented by a coupled set of transport equations, delineates the blood and dialyzate compartments of the hemodialyzer, and includes bicarbonate-buffering reaction in the blood channel and bicarbonate replenishment mechanism in the dialyzate. In a paper submitted by the author, we ignored the inherent velocity discontinuity in the blood channel as the radius of the blood channel r approaches the semi-permeable membrane RB, that is, $r \rightarrow RB$. In this paper, we will investigate the evolution of bicarbonate and carbon dioxide in the blood compartment as the radius of the blood channel approaches the semi-permeable membrane. That is, we will investigate the solutions to the simplified form of the model in the blood compartment near the velocity shock vector, which manifests a discontinuity when $vz(r)=0$ of the simplified non-steady state model. We will investigate the cases of analytical solutions of the model in the blood channel with negligible diffusion and also shock solutions with diffusion.

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GJSFR-F Classification: *MSC 2010: 00A05*

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Global Journal of Science Frontier Research (F) Volume XX Issue VIII Version I Year 2020
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Abstract- Hemodialysis (HD) is one type of procedure for eliminating toxic chemicals and infusing bicarbonate in patients with end-stage renal disease (ESRD). We have developed a comprehensive mathematical model to describe the dynamic exchange process of solutes in a prototype hemodialyzer. The model, which is represented by a coupled set of transport equations, delineates the blood and dialyzate compartments of the hemodialyzer, and includes bicarbonate-buffering reaction in the blood channel and bicarbonate replenishment mechanism in the dialyzate. In a paper submitted by the author, we ignored the inherent velocity discontinuity in the blood channel as the radius of the blood channel r approaches the semi-permeable membrane RB, that is, $r \rightarrow RB$. In this paper, we will investigate the evolution of bicarbonate and carbon dioxide in the blood compartment as the radius of the blood channel approaches the semi-permeable membrane. That is, we will investigate the solutions to the simplified form of the model in the blood compartment near the velocity shock vector, which manifests a discontinuity when $vz(r)=0$ of the simplified non-steady state model. We will investigate the cases of analytical solutions of the model in the blood channel with negligible diffusion and also shock solutions with diffusion.

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I. Introduction

One of the leading goals of HD therapy, aside the elimination of electrolytes, toxic chemicals, and water, is correcting metabolic acidosis by the infusion of bicarbonate as a buffer from the dialyzate into the bloodstream in a prototype hemodialyzer. Normalization of metabolic acidosis sometimes results in, for example, metabolic alkalosis due to over compensation of the acidosis, causing dialysis symptoms such as mental confusion and muscle cramps [1], [2], [3]. Thus, it is of vital importance to obtain the closest if not the exact correction of metabolic acidosis during HD as time progresses.

Research and development in the hemodialyzer technology and HD therapy have depended mostly on empirical evidence. This is costly and often involves numerous clinical trials. In an experiment performed over 12 weeks, Ward et al. [5] were faced with the problem of how to control bicarbonate during HD therapy and that resulted in abnormally high pH value which puts the patient at risk of post-dialytic alkalosis. In an attempt to address the discrepancies in the experimental results, Gotch et al. [4], considered a black box input-output ordinary differential equation model to describe the mass balance of hydrogen ions during HD. Black box model in this case means the internal variables of the hollow fibers were not taken into consideration. Due to variations that were still observed in the experimental results of HD

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Ref

1. Ahmad S, Pagel M, Vizzo J and Scribner BH, Effect of the normalization of acid-base balance on postdialysis plasma bicarbonate, Trans Am Soc Artif Intern Organs 26 (1980) 318-340.

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procedures, there have been increasing need to consider mathematical models. Monti et al. [6] also used a black box input-output ordinary differential equation model to describe the dynamic exchange process of bicarbonate during and after HD. This black-box model was oversimplified because the internal structure and variables of the prototype hemodialyzer unit were not taken into account. Thus, the model did not allow for the prediction of internal variables such as the surface area of the dialyzer, dialyzate flow rates, the thickness and permeability of the membrane [7], [8].

In order to go beyond black-box input-output ordinary differential equation models, and efficiently address the dynamic exchange of solutes in the prototype hemodialyzer, a comprehensive partial differential equation model incorporating internal properties, the dimensions and the surface area of the hollow fibers used during hemodialysis, the nature of solute transfer across the hemodialyzer semi permeable membrane, the hemodialysis flow rates and the duration of the administration of hemodialysis were taken into account. The knowledge gained from this study will eventually lead to a means of predicting the underlying mechanisms of solute transfer in a prototype hemodialyzer, thereby minimizing the need to perform costly and time-consuming clinical trials.

II. Model Description

a) Notation

x Species,
$x = 1: CO_2;\ x = 2: HCO_3^-;\ x = 3: H^+$
ϕ_x Concentration of species in the blood,
$\phi_{0,x}$ Initial concentration of species in the blood,
ψ_x Concentration of species in the dialysate,
$\psi_{0,x}$ Initial concentration of species in the dialysate,
v_z^B Velocity of blood in the axial direction,
v_z^D Velocity of dialyzate in the axial direction,
v_r^B Velocity of blood in the radial direction,
v_r^D Velocity of dialyzate in the radial direction,
v_w^B Wall velocity in the membrane-blood channel,
v_w^D Wall velocity in the membrane-dialyzate channel,
r_B Radius of the blood channel,
r_D Radius of the dialyzate channel,
t_m Membrane thickness,
r_m Sum of t_m and r_B,
S_B Blood-membrane Sherwood number,
S_D Dialyzate-membrane Sherwood number,
Pe_z^B Length Pecle′t number (blood side),
Pe_r^B Radial Pecle′t number (blood side),
Pe_z^D Length Pecle′t number (dialyzate side),
Pe_r^D Radial Pecle′t number (dialyzate side),
L Coaxial entrance length,
B_r Radius of the annulus,
P_x^m Membrane permeability of species,
U_z^B Maximum axial velocity of blood flow,

Ref

6. Monti JP, Sarrazin MY, Baz M, Murisasco A, Crevat AD and Elsen R, Kinetic modeling of intradialytic and interdialytic pH shifts during and after acetate and bicarbonate hemodialysis Int. J Artif. Organs 13 (1990) 799 – 802.

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U_z^D Maximum axial velocity of dialyzate flow,
t_0 Dimensionless time scale,
P_e Pressure at the entrance of the annular,
P_L Pressure at the end of the annular,
$D_{x,r}$ Diffusion coefficient of species in the radial direction,
N_z Axial grid size,
N_r Radial grid size,
N_t Number of tubes,
Q_B Blood flow rate,
Q_D Dialyzate flow rate,
Q_u Ultrafiltration flow rate,
$n(z)$ Mass flux in the blood side channel,
$n(L-z)$ Mass flux in the dialyzate side channel,
B_x The nonlinear reactive term which deals with buffering of the blood,
R_x The replenishment term which replenishes bicarbonate concentration in the dialysate.

b) Model assumptions

We will use the following fundamental assumptions to formulate the models.

- We consider dilute, aqueous and Newtonian flow mechanism in the hemodialyzer.
- We consider permeability, diffusivity and density as constants.
- Axial diffusion was considered negligible.
- Flows were considered laminar.
- The flow mechanisms for the blood and the dialyzate are countercurrent.
- There are no angular gradients (axis-symmetry approximation).

The rate of change of species concentration in the blood and dialyzate channels are given as

$$\frac{\partial \phi_1}{\partial t} + v_z \frac{\partial \phi_1}{\partial z} = D_{r,1} \frac{\partial}{r\partial}\left(r \frac{\partial \phi_1}{\partial r}\right) + B_1 \ , \tag{2.1}$$

and

$$v_z(r) = 2\bar{v}_z \left(1 - \left(\frac{r}{R}\right)^2\right) \tag{2.2}$$

where $D_{r,1}$, $\bar{v}_z$ and v_z are the diffusion coefficient for partial pressure of carbon dioxide, the average velocity, and the axial velocity respectively. In equation (2.1), the second and third terms represent convection and diffusion effects. The initial and boundary conditions of (2.1) and (2.2) are given by

$$\phi_1 = \phi_{1,0} \text{ at } t = 0,\ z > 0; \tag{2.3}$$

$$\phi_1 = \phi_{1,0} \text{ at } t > 0,\ z = 0. \tag{2.4}$$

The condition of no flux at $r = 0$ requires that

$$\frac{\partial \phi_1}{\partial r} = 0. \tag{2.5}$$

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At the blood membrane interface, we write the expression of flux at the boundary $r = R_B$ in the form

$$\frac{-D_{r,1}\partial\phi_1}{\partial r} = P_1^m\phi_1 \ \forall\, z. \tag{2.6}$$

where T_r called the transmittance coefficient is the fraction of solutes that penetrate the membrane pores. Similarly, the convection-diffusion-reaction equation on the dialyzate side is given as

$$\frac{\partial\phi_2}{\partial t} + v_z\frac{\partial\phi_2}{\partial z} = D_{r,2}\frac{\partial}{r\partial}\left(r\frac{\partial\phi_2}{\partial r}\right) + B_2, \tag{2.7}$$

and

$$v_z(r) = 2\bar{v}_z\left(1 - \left(\frac{r}{R}\right)^2\right) \tag{2.8}$$

where $D_{r,1}$, $\bar{v}_z$ and v_z are the diffusion coefficient for bicarbonate, the average velocity, and the axial velocity respectively. In equation (2.7), the second and third terms represent convection and diffusion effects. The initial and boundary conditions of (2.7) and (2.8) are given by

$$\phi_2 = \phi_{2,0} \text{ at } t = 0,\ z > 0; \tag{2.9}$$

$$\phi_2 = \phi_{2,0} \text{ at } t > 0,\ z = 0. \tag{2.10}$$

The condition of no flux at $r = 0$ requires that

$$\frac{\partial\phi_2}{\partial r} = 0. \tag{2.11}$$

At the blood membrane interface, we write the expression of flux at the boundary $r = R_B$ in the form

$$\frac{-D_{r,2}\partial\phi_2}{\partial r} = P_2^m\phi_2 \ \forall\, z. \tag{2.12}$$

For simplicity, we assumed that radial convection is negligible. Since the radius of the blood channel is very small as compared to the length of the tube, we shall assume that the fluid is a fully-formed flow through a semi-infinite hollow fiber where $0 < z < \infty$ and $0 < r < R_B$.

c) Chemical reactions

The most important buffering reaction in the blood is the inter-conversion of CO_2 and HCO_3^-. These undergo the following reversible reaction (catalyzed in the presence of carbonic anhydrase (C.A) or uncatalyzed)

$$CO_2 + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} HCO_3^- + H^+ \tag{Reaction 2.13}$$

where k_1 and k_{-1} are the forward and reversible reaction rate constants respectively. Chemically, (Reaction 2.13) forms a major buffer system of the blood. The net rate of reaction of species by chemical (reaction 2.13) per unit volume can be expressed as

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$$B_x = k_1[CO_2] - k_{-1}[HCO_3^-][H^+] \qquad \text{(Reaction 2.14)}$$

The interrelationship between $pH, HCO_3^-, and\ pCO_2$ is then expressed by the Hendernson-Hasselbalch equation as

$$pH = pK + log_{10}\left(\frac{[HCO_3^-]}{disolved\ CO_2}\right), \qquad (2.15)$$

where $(disolved\ [CO_2] = \alpha pCO_2)$ is the partial pressure of carbon dioxide and α is the solubility constant in $mmol/l$ [9]. The concentration of H^+ is obtained from the pH of the blood by the equation,

$$[H^+] = 10^{-pH} \qquad (2.16)$$

By (Reaction 2.13),

$$B_1 = -k_1[CO_2] + k_{-1}[HCO_3^-][H^+] \qquad (2.17)$$

and

$$B_2 = k_1[CO_2] - k_{-1}[HCO_3^-][H^+] \qquad (2.18)$$

d) Nondimensionalization

We nondimensionalize the models (2.1) to (2.18) by writing

$$\phi_1^* = \frac{\phi_1}{\phi_{1,0}}; \phi_2^* = \frac{\phi_2}{\phi_{2,0}}\ ;\ r^* = \frac{r}{B_r};\ z^* = \frac{z}{L};\ v_z^* = \frac{v_z}{\bar{v}_z};\ t_1^* = \frac{t}{t_{1,0}}; t_2^* = \frac{t}{t_{2,0}}\ ;\ t_{1,0} = \frac{B_r^2}{D_{1,r}};$$

$$t_{2,0} = \frac{B_r^2}{D_{2,r}};\ Pe_1^B = \frac{t_1\bar{v}_z}{L};\ Pe_2^B = \frac{t_2\bar{v}_z}{L}$$

For simplicity, we drop the asterisks to obtain the following nondimensional model and parameters. The dimensionless mass transport model in the blood channel is given as

$$\frac{\partial\phi_1}{\partial t} + Pe_1^B v_z\frac{\partial\phi_1}{\partial z} = D_{r,1}\frac{\partial}{r\partial}\left(r\frac{\partial\phi_1}{\partial r}\right) + t_1(k_{-1}\phi_2\phi_3 - k_1\phi_1), \qquad (2.13)$$

$$\frac{\partial\phi_2}{\partial t} + Pe_2^B v_z\frac{\partial\phi_2}{\partial z} = D_{r,2}\frac{\partial}{r\partial}\left(r\frac{\partial\phi_2}{\partial r}\right) - t_2(k_{-1}\phi_2\phi_3 - k_1\phi_1), \qquad (2.14)$$

$$v_z(r) = 2(1 - r^2)\,, \qquad (2.15)$$

$$B_1 = -t_0k_1\left(\alpha\phi_1 - \frac{\phi_2}{10^{pH}K}\right) \qquad (2.16)$$

and

$$B_2 = k_1\left(\alpha\phi_1 - \frac{\phi_2}{10^{pH}K}\right) \qquad (2.17)$$

where $K = \frac{k_1}{k_{-1}}\ and\ B_3 = 0$. The concentration of hydrogen ions in the blood in (2.13) and (2.14) may be simplified as

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$$\phi_3 = \frac{\alpha\phi_1}{10^{pK}\phi_2}. \tag{2.18}$$

Thus, the reaction terms containing ϕ_3 are simplified as

$$\pm t_{1,2}(k_{-1}\phi_2\phi_3 - k_1\phi_1) = \pm\beta_{1,2}\phi_1, \tag{2.19}$$

where $\pm t_{1,2}k_1\left(\frac{\alpha-10^{pK}K}{10^{pK}K}\right)$. The dimensionless, initial, boundary and no-flux conditions and the interfacial membrane relations are given as follows:

Boundary conditions:

$$\phi_1(z,r,0) = \phi_2(z,r,0) = 1,\ z > 0, \tag{2.20}$$

$$\phi_1(0,r,t) = \phi_2(0,r,t) = 1,\ t > 0, \tag{2.21}$$

No-flux conditions:

$$\frac{\partial\phi_1(z,0,t)}{\partial r} = \frac{\partial\phi_2(z,0,t)}{\partial r} = 0, \tag{2.22}$$

Interfacial membrane relations:

$$-\frac{D_{r,1}\partial\phi_1(z,1,t)}{\partial r} = sh_1\phi_1 \tag{2.23}$$

$$-\frac{D_{r,2}\partial\phi_1(z,1,t)}{\partial r} = sh_2\phi_2 \tag{2.24}$$

where $sh_1 = \frac{P_{m,1}R_B}{D_{r,1}}$ and $sh_2 = \frac{P_{m,2}R_B}{D_{r,2}}$. The dimensionless model in (2.13) to (2.15) may be written as.

$$\frac{1}{Pe_1^B}\frac{\partial\phi_1}{\partial t} + v_z\frac{\partial\phi_1}{\partial z} = D_{r,1}\frac{\partial}{Pe_1^B r\partial}\left(r\frac{\partial\phi_1}{\partial r}\right) + \frac{\beta\phi_1}{Pe_1^B}, \tag{2.25}$$

$$\frac{1}{Pe_2^B}\frac{\partial\phi_2}{\partial t} + v_z\frac{\partial\phi_2}{\partial z} = D_{r,2}\frac{\partial}{Pe_2^B r\partial}\left(r\frac{\partial\phi_2}{\partial r}\right) - \frac{\beta\phi_1}{Pe_2^B}, \tag{2.26}$$

with the initial and boundary conditions as given in (2.20) and (2.21).

III. The Solution Without Diffusion

As a first approximation, we neglect the diffusion and the time derivative terms in (2.25) and (2.26) since $\frac{1}{Pe_1^B} = \frac{1}{Pe_2^B} \approx 1$ and so the reduced equations are given as

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$$v_z \frac{\partial \phi_1}{\partial z} = \frac{\beta \phi_1}{Pe_1^B}, \tag{2.27}$$

$$v_z \frac{\partial \phi_2}{\partial z} = \frac{\beta \phi_1}{Pe_2^B}, \tag{2.28}$$

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together with the given boundary conditions. Since v_z is a function of only r, we may use the transformation

$$X = \frac{zt}{v_z(r)}, \tag{2.29}$$

and so equations (2.27) and (2.28) become

$$\frac{\partial \phi_1}{\partial X} = \frac{\beta}{tPe_1^B}\phi_1, \tag{2.30}$$

$$\frac{\partial \phi_2}{\partial X} = \frac{\beta}{Pe_2^B}\phi_1, \tag{2.31}$$

$$\phi_1(0,r,t) = 1, t > 0 \text{ becomes } \phi_1 = 1 \text{ at } X = 0,$$

$$\phi_2(0,r,t) = 1, t > 0 \text{ becomes } \phi_2 = 1 \text{ at } X = 0.$$

The solutions to the problems in (2.30) to (2.31) are given as

$$\phi_1 = exp\left(\frac{\beta}{tPe_1^B}X\right) = exp\left(\frac{\beta z}{v_z Pe_1^B}\right) \tag{2.32}$$

$$\phi_2 = 1 + \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta}{tPe_1^B}X\right)\right) = 1 + \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta z}{v_z Pe_1^B}\right)\right) \tag{2.33}$$

The solutions in (2.30) and (2.31) satisfy the boundary conditions on $X = 0$, but physically, this is not significantly interesting. We are rather interested in the observation away from $z = 0$.

IV. The Solution with Diffusion

Using the approximation, $\frac{1}{Pe_1^B} \approx \frac{1}{Pe_2^B} \approx \frac{\beta}{Pe_1^B} \approx \frac{\beta}{Pe_2^B} = \varepsilon \ll 1$, we retain the diffusion terms in (2.25) and (2.26) and perform the computational analysis to examine the behavior of species concentrations near the membrane boundary. We may write,

$$\frac{1}{Pe_1^B}\frac{\partial \phi_1}{\partial t} + v_z \frac{\partial \phi_1}{\partial z} = D_{r,1}\frac{\partial}{Pe_1^B r \partial}\left(r\frac{\partial \phi_1}{\partial r}\right) + \frac{\beta \phi_1}{Pe_1^B}, \tag{2.34}$$

$$\frac{1}{Pe_2^B}\frac{\partial \phi_2}{\partial t} + v_z \frac{\partial \phi_2}{\partial z} = D_{r,2}\frac{\partial}{Pe_2^B r \partial}\left(r\frac{\partial \phi_2}{\partial r}\right) - \frac{\beta \phi_1}{Pe_2^B}, \tag{2.35}$$

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where $\frac{1}{Pe_1^B} \approx \frac{1}{Pe_2^B} \approx \frac{\beta}{Pe_1^B} \approx \frac{\beta}{Pe_2^B} \ll 1$

We require that the solutions for (2.34) and (2.35) satisfy the given dimensionless boundary conditions. Now, we study the behavior of solute transfer near the shock $z = 2(1 - r^2)t$. Thus, we introduce the new variables

$$\xi = z - v_z(r)t, \;\; \eta = r, \;\; \tau = t \tag{2.36}$$

to transform the differential equations in (2.34) and (2.35) as follows:

$$\frac{\partial \phi_1}{\partial t} = \frac{\partial \xi}{\partial t}\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \eta}{\partial t}\frac{\partial \phi_1}{\partial \eta}, + \frac{\partial \tau}{\partial t}\frac{\partial \phi_1}{\partial \tau} \tag{2.37}$$

$$\frac{\partial \phi_1}{\partial t} = -v_z(\eta)\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \phi_1}{\partial \tau} \tag{2.38}$$

Also,

$$\frac{\partial \phi_1}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial \phi_1}{\partial \eta}, + \frac{\partial \tau}{\partial x}\frac{\partial \phi_1}{\partial \tau} \tag{2.39}$$

$$v_z(r)\frac{\partial \phi_1}{\partial x} = v_z(\eta)\frac{\partial \phi_1}{\partial \xi} \tag{2.40}$$

and finally,

$$\frac{\partial \phi_1}{\partial r} = \frac{\partial \xi}{\partial r}\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \eta}{\partial r}\frac{\partial \phi_1}{\partial \eta}, + \frac{\partial \tau}{\partial r}\frac{\partial \phi_1}{\partial \tau} \tag{2.41}$$

$$\frac{\partial \phi_1}{\partial r} = 2\eta\tau\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \phi_1}{\partial \eta}, \tag{2.42}$$

from which it follows that

$$\frac{\partial^2 \phi_1}{\partial r^2} = 4\tau^2\eta^2\frac{\partial^2 \phi_1}{\partial \xi^2} + 4\tau\eta\frac{\partial^2 \phi_1}{\partial \xi \partial \eta} + 2\tau\frac{\partial \phi_1}{\partial \xi} + \frac{\partial^2 \phi_1}{\partial \eta^2}. \tag{2.43}$$

Substituting (2.38), (2.40), (2.42) and (2.43) into (2.34) to (2.35) and simplifying, we obtain

$$\frac{\partial \phi_1}{\partial \tau} = \frac{1}{Pe_1^B}\left(4\tau^2\eta^2\frac{\partial^2 \phi_1}{\partial \xi^2} - 4\tau\eta\frac{\partial^2 \phi_1}{\partial \xi \partial \eta} - 4\tau\frac{\partial \phi_1}{\partial \xi} + \frac{\partial \phi_1}{\eta \partial \xi} + \frac{\partial^2 \phi_1}{\partial \eta^2}\right) + \frac{\beta \phi_1}{Pe_1^B} \tag{2.44}$$

$$\frac{\partial \phi_2}{\partial \tau} = \frac{1}{Pe_2^B}\left(4\tau^2\eta^2\frac{\partial^2 \phi_2}{\partial \xi^2} - 4\tau\eta\frac{\partial^2 \phi_2}{\partial \xi \partial \eta} - 4\tau\frac{\partial \phi_2}{\partial \xi} + \frac{\partial \phi_2}{\eta \partial \xi} + \frac{\partial^2 \phi_2}{\partial \eta^2}\right) + \frac{\beta \phi_2}{Pe_2^B} \tag{2.45}$$

For simplicity, we transform equations (2.44) and (2.45) by using

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$$\xi = \frac{X}{\sqrt{Pe_{1,2}^{B}}} \tag{2.46}$$

and use the outer solutions from the previous section so that

$$\phi_1 = \phi_2 = 1 \tag{2.47}$$

Notes

and

$$\phi_1 = exp\left(\frac{\beta}{\tau Pe_1^B} X\right), \quad \phi_2 = 1 - \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta}{\tau Pe_1^B} X\right)\right), \quad \xi > 0 \tag{2.48}$$

This choice of transformation in (2.46) helps to simplify and remove fractions from the system. We substitute (2.46) into equations (2.44) and (2.45) and simplify to obtain

$$\frac{\partial \phi_1}{\partial \tau} = 4\tau^2\eta^2 \frac{\partial^2 \phi_1}{\partial X^2} + \varepsilon\phi_1 + O\left(\mu, \frac{1}{\sqrt{Pe_1^B}}\right) \tag{2.49}$$

$$\frac{\partial \phi_2}{\partial \tau} = 4\tau^2\eta^2 \frac{\partial^2 \phi_2}{\partial X^2} - \varepsilon\phi_1 + O\left(\mu, \frac{1}{\sqrt{Pe_2^B}}\right) \tag{2.50}$$

The following are the associated boundary conditions:

$$\phi_1 \to 1 \text{ as } X \to -\infty \tag{2.51}$$

$$\phi_1 \to exp\left(\frac{\beta}{\tau Pe_1^B} X\right) \text{ as } X \to +\infty \tag{2.52}$$

$$\phi_1 \to 1 \text{ as } \tau \to 0, \tag{2.53}$$

and

$$\phi_2 \to 1 \text{ as } X \to -\infty \tag{2.54}$$

$$\phi_2 \to 1 - \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta}{\tau Pe_1^B} X\right)\right) \text{ as } X \to +\infty \tag{2.55}$$

$$\phi_2 \to 1 \text{ as } \tau \to 0\,. \tag{2.56}$$

We may now apply the method of multiple scales (Nayfeh, 1973) to solve (2.49) to (2.56) with $\varepsilon \ll 1$ and $\mu \ll 1$. We introduce the fast time $T_0 = t$ and the slow time $T = \varepsilon t$ for (2.49) and (2.50). Expanding the solutions to (2.49) and (2.50) as

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$$\phi_{1,2}(X,T) = \phi_{1,2}^{(0)}(X,T_0,T_1) + \phi_{1,2}^{(1)}(X,T_0,T_1) + \cdots, \tag{2.57}$$

and substituting $\phi_1^{(0)}$ will yield

$$\frac{\partial \phi_{1,2}^{(0)}}{\partial T_0} = 4\eta^2 T_0^2 \frac{\partial^2 \phi_{1,2}^{(0)}}{\partial X^2}, \tag{2.58}$$

$$\phi_{1,2}^{(0)} \to 1 \text{ as } X \to -\infty, \tag{2.59}$$

$$\phi_{1,2} \to 1 + exp\left(\frac{\beta}{Pe_1^B}X\right), 1 - \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta}{Pe_1^B}X\right)\right) \text{ as } X \to +\infty, \tag{2.60}$$

$$\phi_{1,2}^{(0)} \to 1 \text{ as } T_0, T_1 \to -\infty. \tag{2.61}$$

We define a new variable that combines both X and T_0 in the form

$$\rho = \frac{\sqrt{3}}{4\eta T_0^{\frac{3}{2}}}X, \tag{2.62}$$

and then convert the derivatives of $\frac{\partial}{\partial \tau}$ and $\frac{\partial}{\partial X}$ to $\frac{\partial}{\partial T_0}$ and $\frac{\partial}{\partial \rho}$ respectively to obtain

$$\frac{\partial \phi_{1,2}^{(0)}}{\partial T_0} = -\frac{3\sqrt{3}}{8\eta T_0^{\frac{5}{2}}}X\frac{\partial \phi_{1,2}}{\partial \rho}, \tag{2.63}$$

and

$$\frac{\partial^2 \phi_2}{\partial X^2} = -\frac{3}{16\eta^2 T_0^3}X\frac{\partial^2 \phi_{1,2}}{\partial \rho^2}. \tag{2.64}$$

Substituting, (2.58) will become

$$-2\left(\frac{X\sqrt{3}}{4\eta T_0^{\frac{3}{2}}}\right)\frac{\partial \phi_{1,2}}{\partial \rho} = \frac{\partial^2 \phi_{1,2}}{\partial \rho^2}, \tag{2.65}$$

which is simplified to the form

$$\frac{\partial^2 \phi_{1,2}}{\partial \rho^2} + 2\rho\frac{\partial \phi_{1,2}}{\partial \rho} = 0, \tag{2.65}$$

Since was defined such that $\rho = \frac{\sqrt{3}}{4\eta T_0^{\frac{3}{2}}}X$. Here, we note that the original differential equation for $\phi_{1,2}(\tau, X)$ has been transformed to an equation for $\phi_{1,2}(\rho)$ with boundary conditions given as follows:

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$$\phi_{1,2}^{(0)} \to 1 \text{ as } X \to -\infty \text{ will become } \phi_{1,2}^{(0)} \to 1 \text{ as } \rho \to \infty \tag{2.66}$$

$$\phi_{1,2}^{(0)} \to 1 \text{ as } T_0, T_1 \to -\infty \text{ will become } \phi_{1,2}^{(0)} \to 1 \text{ as } \rho \to \infty \tag{2.67}$$

Notes

and equation (2.60) will also be transformed to the corresponding matching condition. We note that the two boundary conditions in τ and X collapse to a single boundary condition on ρ. In summary, we have transformed the partial differential equations and the corresponding boundary conditions to the form

$$\frac{\partial^2 \phi_{1,2}^{(0)}}{\partial \rho^2} + 2\rho \frac{\partial \phi_{1,2}^{(0)}}{\partial \rho} = 0, \tag{2.68}$$

$$\phi_{1,2}^{(0)} \to 1 \text{ as } \rho \to \infty, \tag{2.69}$$

$$\phi_{1,2}^{(0)} \to 1 + exp\left(\frac{\beta}{tPe_1^B} X\right), 1 - \frac{Pe_1^B}{Pe_2^B}\left(1 - exp\left(\frac{\beta}{Pe_1^B} X\right)\right) \text{ as } X \to \infty, \tag{2.70}$$

Since the only variable appearing in the partial differential equation is ρ, we conclude that $\phi_{1,2}^{(0)} = \phi_{1,2}^{(0)}(\rho)$ and the new equation is an ordinary differential equation of the form

$$\frac{d^2 \phi_{1,2}^{(0)}}{\partial \rho^2} + 2\rho \frac{d\phi_{1,2}^{(0)}}{d\rho} = 0 \tag{2.71}$$

with the given boundary conditions. We solve (2.71) by denoting and substituting $\frac{d\phi_{1,2}^{(0)}}{d\rho} = f$ to obtain

$$\frac{df}{d\rho} + 2\rho f = 0. \tag{2.72}$$

Solving (2.72), we obtain

$$f = f_0 e^{-\rho^2} \text{ and so } \frac{d\phi_{1,2}}{d\rho} = f_0 e^{-\rho^2} \tag{2.73}$$

which implies

$$\phi_{1,2} = \frac{f_0}{\sqrt{\pi}} \int_{-\infty}^{\rho} e^{-\lambda^2}\, d\lambda \tag{2.74}$$

$$\phi_{1,2} = \frac{f_{0,1,2}}{\sqrt{\pi}} \int_{-\infty}^{\frac{\sqrt{3}X}{4\eta T_0^{3/2}}} e^{-\lambda^2}\, d\lambda \tag{2.75}$$

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We apply the corresponding boundary conditions and rewrite (2.75) in terms of original variables to obtain first order solutions that are uniformly valid in the forms

$$\phi_1 = \frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{\sqrt{\pi}}\int_{-\infty}^{\frac{\sqrt{3Pe_1^B}(z-v_z t)}{4rt^{3/2}}} e^{-\lambda^2}d\lambda + O\left(\varepsilon, 1/\sqrt{Pe_1^B}, \mu\right) \tag{2.76}$$

$$\phi_1 \approx \frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{\sqrt{\pi}}\left(\int_{-\infty}^{0} e^{-\lambda^2}d\lambda + \int_{0}^{\frac{\sqrt{3Pe_1^B}(z-v_z t)}{4rt^{3/2}}} e^{-\lambda^2}d\lambda\right), \tag{2.77}$$

$$= \frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{2\sqrt{\pi}}\left(\sqrt{\pi} + \frac{2}{\sqrt{\pi}}\int_{0}^{\frac{\sqrt{3Pe_1^B}(z-v_z t)}{4rt^{3/2}}} e^{-\lambda^2}d\lambda\right), \tag{2.78}$$

$$\phi_1 = \frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{2\sqrt{\pi}}\left(\sqrt{\pi} + erf\left(\sqrt{3Pe_1^B}\left(\frac{Z-V_z t}{4rt^{3/2}}\right)\right)\right), \tag{2.79}$$

Similarly,

$$\phi_2 = \left(\frac{Pe_1^B+Pe_2^B}{Pe_2^B}\right)\frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{\sqrt{\pi}}\int_{-\infty}^{\frac{\sqrt{3Pe_1^B}(z-v_z t)}{4rt^{3/2}}} e^{-\lambda^2}d\lambda + O\left(\varepsilon, 1/\sqrt{Pe_2^B}, \mu\right) \tag{2.80}$$

which implies

$$\phi_2 \approx \left(\left(\frac{Pe_1^B+Pe_2^B}{Pe_2^B}\right)\left(\frac{1+exp\left(\frac{\beta}{Pe_1^B}X\right)}{2\sqrt{\pi}}\right)\right)\left(\sqrt{\pi} + erf\left(\sqrt{3Pe_1^B}\left(\frac{Z-v_z t}{4rt^{3/2}}\right)\right)\right) \tag{2.81}$$

V. Concluding Remarks

We considered the evolution of solute concentrations in the blood compartment during HD therapy by solving the model when diffusion coefficients were negligible. On the other hand, a small but non zero diffusion coefficients, were introduced and as a result, the solutions were modified by smoothing out the discontinuity present as r approaches the membrane in the blood compartment. Equations 2.78 – 2.81 are explicit solutions of the dimensionless concentrations of bicarbonate and partial pressure of carbon dioxide as $r \to R_B$ in the blood compartment. The results we observed were solute concentrations as functions of time and distances specified along the hollow fiber. The result might help to give more insight into the change of solute concentration as diffusion across the semi-permeable membrane occurs.

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We have proposed and given analytical results of the modified model system for bicarbonate HD which may practically be used. The theoretical model presented provides valuable insight into the system characteristics and serves as a rational basis for interpreting data.

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