Modeling Dialysis

By: Kevin Chen, Samson Fong, and Avi Kumar

Table of Contents

Introduction

Healthy kidneys are vital organs in the body. The kidneys filter toxins, such as urea and creatinine, out of the bloodstream as well as balance the pH, and water level in the bloodstream. They also regulate blood pressure. Mass transfer in the kidneys occurs through the one million nephrons located in each kidney. As shown in Figure 1, unfiltered blood enters the nephrons and reaches the glomerulus where the toxins are filtered into the tubule and out of the body through the urine. Filtered blood returns to the bloodstream. The entire content of circulatory system is typically filtered every 30 to 60 minutes in humans, depending on the subjects resting heart rate. (1)

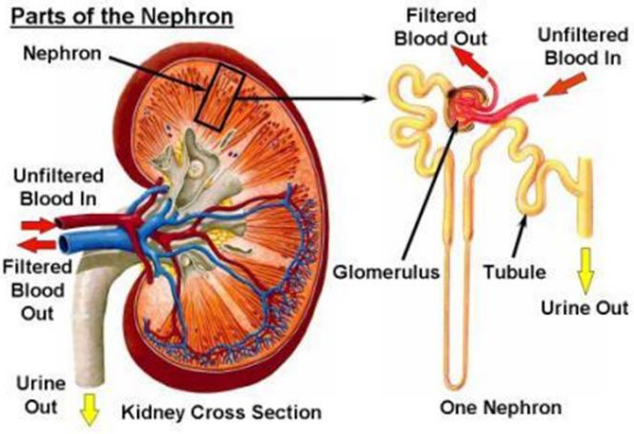

Figure 1: Kidney Anatomy (2)

Kidney disease is the result of poor mass transfer in the nephrons. It is caused by a variety of maladies including poor diet, diabetes, and overuse of pain medications. Nearly 1 in 3 Americans is at risk for the disease and 26 million Americans have it. Beyond a transplant, there is no cure for kidney disease and; as a result, it is the 9th leading cause of death in the United States. The most common treatment for kidney disease is dialysis. Nearly 500,000 Americans are currently on dialysis. And although popular, it is not a convenient therapy, requiring up to 8 hour sessions 5 to 7 days a week. (3)

There are two types of dialysis, peritoneal dialysis and hemodialysis. Peritoneal dialysis involves inserting a dialysate fluid directly into the body to capture toxins from the bloodstream for a set amount of time before the fluid is removed. Hemodialysis, which is much more common in the U.S., involves external mass transfer of toxins from the blood stream via a dialyzer. A dialyzer operates essentially as an artificial kidney as shown in Figure 2. Blood is pumped from the patient, through hollow fibers in the dialyzer. The hollow fibers are surrounded by a semipermeable membrane which allows for mass transfer of small molecules such as urea from the blood to the dialysate, which is pumped counter-currently across the outside of the blood containing tubes. Dialysis sessions are so time intensive because the entire blood volume of the patient must be flown through the dialyzer multiple times, until toxin levels are minimal. Dialysis must be performed nearly daily as toxins are continuously produced in the bloodstream, and their levels must be controlled to avoid potentially lethal effects. (4)

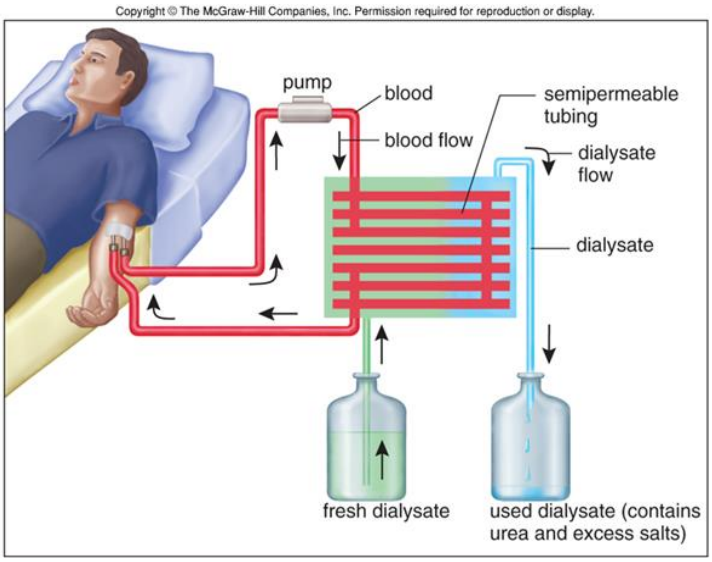

Figure 2: Simplified Dialyzer Flow Diagram (5)

Problem Statement

The objective of this work is to develop a full-fledged model of a dialyzer which can be used to for dialyzer design. A diagram of the full model is shown in Figure 3. Both blood and countercurrent dialysate flow and concentrations will be included in the model. The model needs to account for mass transfer in the z direction in the tube and both the z and radial directions in the membrane. Additionally, a macroscopic model of the dialyzer will look at mass transfer over the length of the dialyzer over time, in order to model the number of circulations through the dialyzer required to reduce urea levels in the blood stream. Urea will be used as the model analyte.

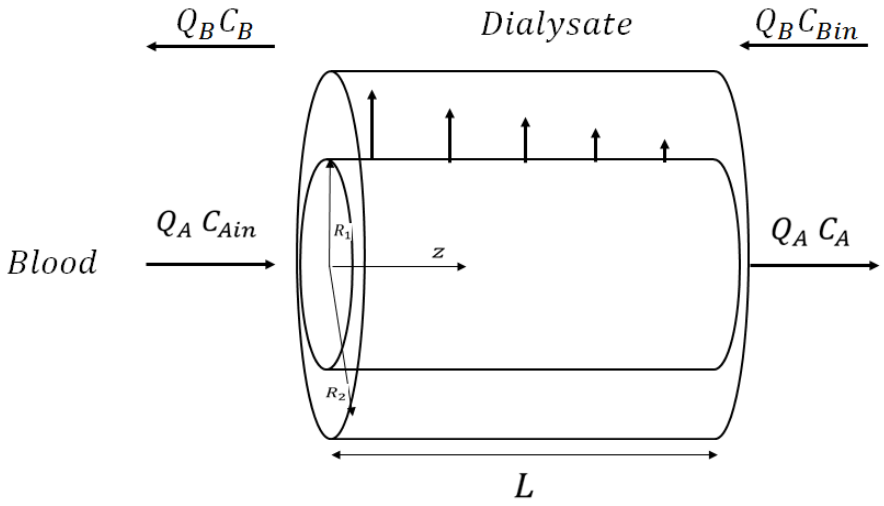

Figure 3: Diagram of Dialyzer. The outer cylinder represents the membrane and its width (not to scale). The dialysate shown as the outer compartment (not drawn).

Methods

To design the model, the problem can be broken down into multiple pieces. In case 1, the problem is simplified by considering only a cross section of the system of interest. By doing so, the variation in the length of the pipe is ignored. This case will focus on the dynamics of the bulk fluid within the blood vessel in the dialysate. To look at the bulk movement of urea from the blood vessel compartment to the dialysate, the model will assume the mass transfer equation,

$$N = k(c_{1,i} - c_1)$$

where N is the flux across a vessel, $c_{1,i}$ is the concentration on one interface, and c_i is the concentration at the other interface. The mass transfer coefficient "expects that the amount transferred is proportional to the concentration difference and the interfacial area…where the proportionality is summarized by k, called a mass transfer coefficient" (6).

This equation is widely used, especially in chemical engineering, to experimentally fit a coefficient to this proportionality. The mass transfer equation has the advantage of ignoring the geometry of the vessel, simplifying the problem. While this equation is very similar to the 1-D diffusion equation that arises from Fick's law in Cartesian coordinates, it is meant to be used more as a fitting parameter in practice. A more rigorous derivation will be demonstrated in later cases.

In case 2, the dynamics within the membrane are considered. In cases 3 and 4, the entire system is considered. Specifically, case 3 deals with the dynamics of the blood vessel and considers how concentration changes along the z-direction. In case 4, the concentration profile within the membrane along the radial component and z-component is evaluated. In order to develop the governing equation, a mass balance was performed on a control volume. This theoretically provides a solution that explains the concentration gradient in the length, radial, and time dimensions.

Results

Case 1

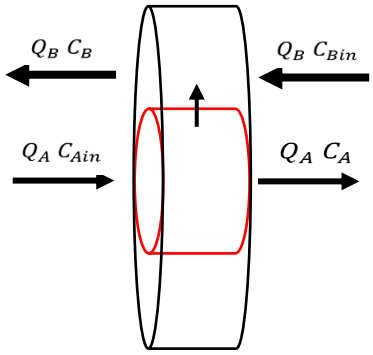

Figure 4: Shows the slice of the system.

Since this case ignores the dynamics within the membrane, the membrane thickness is ignored in the diagram. The blood vessel is shown in red with volumetric flow rate Q_a and uniform concentration C_a. The blood urea concentration is assumed to be constant at the inlet, C_{ain}. The concentration at the slice changes only with time (no radial gradient). Similarly, the dialysate

volumetric flow rate is Q_b, with uniform inlet concentration C_{bin}. Although the concentration should be zero, as the dialysate enters the dialyzer free of toxins, the term is carried for completeness. A mass balance results in the following system of equations.

$$V_A \frac{dC_A}{dt} = Q_A(C_{Ain} - C_A) - K(C_A - C_B)$$

$$V_B \frac{dC_B}{dt} = Q_B(C_{Bin} - C_B) + K(C_A - C_B)$$

$$C_A(0) = C_{Ain} \qquad C_B(0) = C_{Bin}$$

V_a and V_b refer to the volume of the blood vessel and the dialysate compartment respectively. The first term in both equations represent the flow in and out of the pipes while the $k(C_a - C_b)$ term represents the bulk urea movement from the vessel to the dialysate (see discussion of mass transfer coefficient). In cases 3 and 4, the model will be expanded to include variations in the spatial dimensions as well.

The system of equations can be solved analytically by turning the system of equations into a matrix equation (below) and is solved by constructing the sum of corresponding homogenous and particular solutions using the steady state solution.

$$\begin{bmatrix} \frac{dC_A}{dt} \\ \frac{dC_B}{dt} \end{bmatrix} = \begin{bmatrix} V_A + K & -K \\ -K & V_B + K \end{bmatrix} \begin{bmatrix} C_A \\ C_B \end{bmatrix} + \begin{bmatrix} C_{Ain}Q_A \\ C_{Bin}Q_B \end{bmatrix}$$

$$u(t) = u_H(t) + u_p(t)$$

The homogeneous solution can be solved using eigenvalue analysis and finding the corresponding eigenvectors.

$$\begin{bmatrix} \frac{dC_A}{dt} \\ \frac{dC_B}{dt} \end{bmatrix} = \begin{bmatrix} V_A + K & -K \\ -K & V_B + K \end{bmatrix} \begin{bmatrix} C_A \\ C_B \end{bmatrix}$$

$$\begin{bmatrix} C_{A,H} \\ C_{B,H} \end{bmatrix} = \begin{bmatrix} \eta_{1,1} \\ \eta_{1,2} \end{bmatrix} Ae^{\lambda_1 t} + \begin{bmatrix} \eta_{2,1} \\ \eta_{2,2} \end{bmatrix} Be^{\lambda_2 t}$$

The steady state solution implies no time dependence in the equations which turn the time derivatives into the zero vector. The resulting set of linear equations can be solved using matrix inversions.

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} V_A + K & -K \\ -K & V_B + K \end{bmatrix} \begin{bmatrix} C_A \\ C_B \end{bmatrix} + \begin{bmatrix} C_{Ain}Q_A \\ C_{Bin}Q_B \end{bmatrix}$$

$$\begin{bmatrix} C_{A,P} \\ C_{B,P} \end{bmatrix} = \begin{bmatrix} C_{A,SS} \\ C_{B,SS} \end{bmatrix}$$

The following equation shows the sum final solution once the constants were substituted in (Supplement).

$$\begin{bmatrix} C_{A,H} \\ C_{B,H} \end{bmatrix} = \begin{bmatrix} 0.27 \\ -0.29 \end{bmatrix} e^{-30.9t} + \begin{bmatrix} 0.043 \\ 0.040 \end{bmatrix} e^{-7.47t} + \begin{bmatrix} 0.43 \\ 0.25 \end{bmatrix}$$

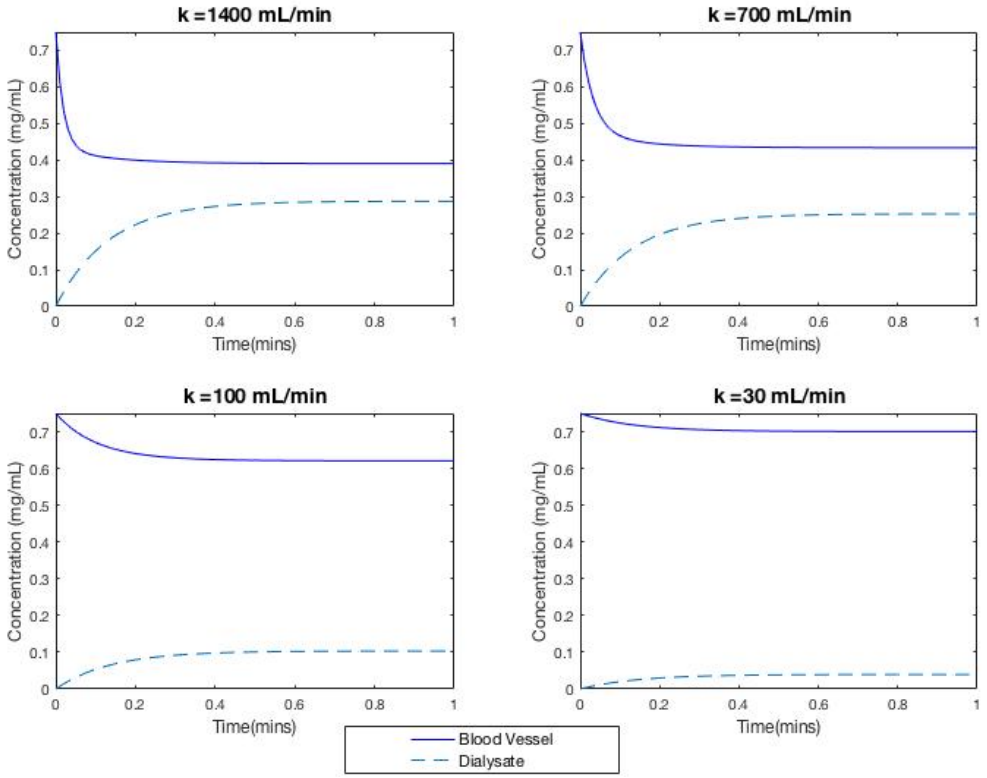

Figure 5: Shows the exponential decay behavior of both compartments. Solid line represents the concentration in the blood vessel compartment, and the dotted line represents the concentration in the dialysate compartment.

The concentration within both compartments reach some steady state value. At this point, the mass transfer is complete, and no more purification can be achieved. This point signals that the amount of urea entering the blood vessel equals to the sum of the amount of urea diffusing into the dialysate and out of the blood vessel. Since the steady state solution does not reach a desirable level of urea, the outlet blood will need to be passed back as the input, a practice commonly performed in dialysis treatment (4).

Figure 5 shows the effect of the mass transfer coefficient on the concentration profiles in both compartments. A lower coefficient corresponds to less mass transfer across the membrane, resulting in more urea staying in the blood vessel. As a result, the lower coefficient leads to a significantly higher concentration, in the blood vessel, at steady state.

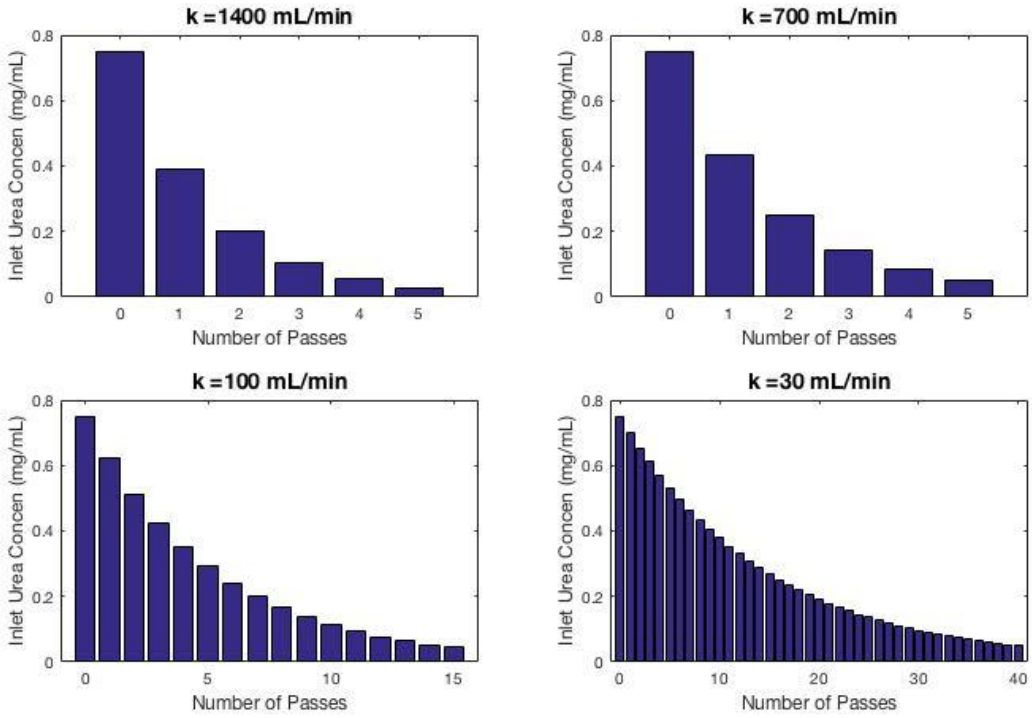

Figure 6: Shows the relationship between the number of passes and the blood vessel concentration.

Figure 6 shows the number of passes the system requires to reach an acceptable level of urea in the blood vessel (0.05 mg/mL) (7). By lowering the driving force (lower *k*), mass transfer occurs less quickly, and the steady state mass balance occurs at a higher concentration as seen in Figure 5. This means each pass of the dialysis is not very effective, leading to a significantly higher number of passes needed.

Furthermore, Figure 6 also demonstrates the primary obstacle in many purification systems. As the concentration of the fluid becomes lower and lower due to the separation, the driving force that pushes the substance of interest also lowers leading to less efficient purification with every pass. This can be seen in the exponential decay of the figure.

Case 2

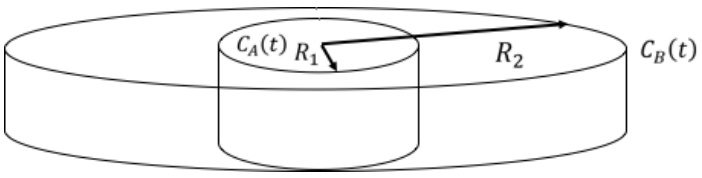

Figure 7: This is a similar system to case 1, but the membrane is expanded to show the width of the membrane. The scale is exaggerated to display the membrane more clearly.

In the second case, the membrane dynamics are considered for the same system as case 1. Since the diffusion is only in the radial direction, the problem simplifies to a 1-D diffusion problem in cylindrical coordinates.

$$\frac{\partial C_M}{\partial t} = D\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)$$

$$I.C.\ \ @\, t = 0,\ \ C_M(r,0) = 0$$

$$B.C.\ \ @\, r = R_1,\ \ C_M(R_1,t) = C_A(t)$$

$$B.C.\ \ @\, r = R_2,\ \ C_M(R_2,t) = C_B(t)$$

The initial condition assumes that the membrane contains no urea anywhere in the membrane. The boundary conditions for the membrane were determined in case 1, as the boundary concentrations are simply the urea concentration in the blood vessel and dialysate as a function of time. While the differential equation is simple, the exponential equations of the boundaries make solving for the analytical solution very complicated. However, this problem can be solved simply using Matlab's pdepe function.

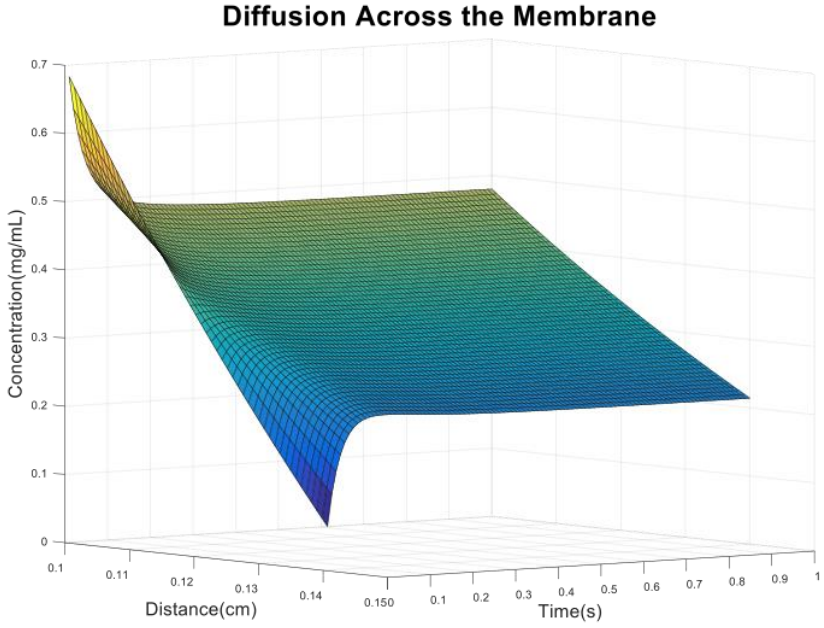

Figure 8: Matlab's pdepe result of 1-D cylindrical coordinate diffusion. The result shows the expected exponential functions at the boundaries.

The plot shows the exponential curves of the boundary conditions as specified above. Most of the nonlinear dynamics occur at the early transient time scale as both boundaries are rapidly changing in concentration. At steady state, the diffusion across the membrane occurs nearly linearly. However, this is not exactly the case due to the cylindrical coordinate system. This will be explored further in case 4.

Case 3

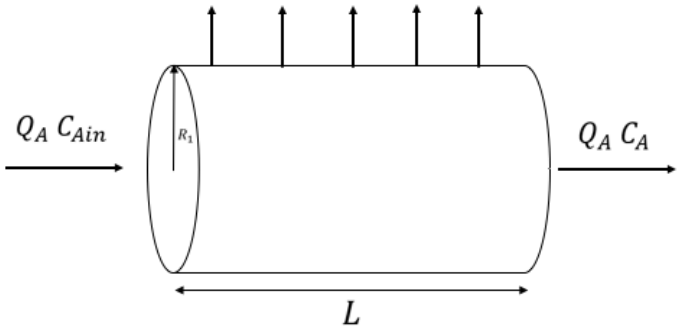

Figure 9: The diagram shows the length of the tube as well as the diffusion across the membrane (width not drawn explicitly).

In the final cases the concentration profile along the length of the dialyzer was explored. Performing a mass balance across a small length of the blood vessel produces the following equation:

$$V\frac{dC}{dt} = QC|_z - QC|_{z+\Delta z} - \left(AJ|_{r=R_1}\right)$$

Where *V* is the volume of the blood vessel, *Q* is the volumetric flow of blood, *A* is the surface area of the blood vessel, and *J* is the flux at the wall of the blood vessel. It is assumed that the concentration is constant in each slice of *z* within the blood vessel. In other words, there is no radial component of *C* within the blood vessel.

The volume, volumetric flow rate, and area can be further broken down in terms of ***Δz***:

$$\pi R^2\Delta z\frac{\partial C(z,t)}{\partial t} = \pi R^2 vc(z,t) - \ \pi R^2 vc(z+\Delta z,\ t) - \ 2\pi R\Delta z(-D\frac{\partial C}{\partial r})$$

Here, *v* is the velocity of the blood. The velocity is assumed to be constant in the radial direction. This assumption is made to simplify the model (see discussion of the radial component in the Discussion section). Dividing by the volume, results in the following equation:

$$\frac{dC}{dt} = v\frac{C|_z - C|_{z+\Delta z}}{\Delta z} + (\frac{2D}{R_1} * \frac{dC}{dr}|_{r=R_1})$$

Which simplifies to:

$$\frac{dC}{dt} = v\frac{-dC}{dz} + (\frac{2D}{R_1} * \frac{dC}{dr}|_{r=R_1})$$

This governing equation is a first order hyperbolic partial differential equation. Unfortunately, this cannot be solved using Matlab's pdepe since the function expects a second order, one-dimensional differential equation. However, here it is important to note that we are interested in the steady-state behavior of our system, instead of startup flux through the membrane. We want to know how much of the urea is filtered out once the blood passes through the entirety of the membrane region at steady state. This will simplify the problem by since there is no longer any time-dependence,

$$v\frac{dC}{dz} = \left(\frac{2D}{R_1} * \frac{dC}{dr}|_{r=R_1}\right)$$

The values for the bulk velocity of the blood and the radius of the blood vessel are taken from literature. The dialysate concentration is approximated to equal 0 across all z as the volumetric flow rate is high and it enters the dialyzer in a pure state.

The flux at the wall of the blood vessel is influenced by the diffusion of urea across the membrane. Solving for steady-state diffusion in the membrane gives the following equation:

$$0 = D\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)$$

With boundary conditions $C(R_2)=0$ and $C(R_1)=C_0$. The solution is of the form

$$C = Aln(r) + B$$

The flux is then given by:

$$\frac{dC}{dr} = \frac{A}{r}; A = \frac{C_0}{\ln\left(\frac{R_1}{R_2}\right)}$$

Plugging this back into our mass balance in the blood vessel,

$$\frac{dC}{dz} = M * C, \text{ where } M = \frac{2D}{vR_1^2\ln(R_1/R_2)}$$

A solution of this first order ode is $C = C_0\exp(-Mz)$ and the graphs are displayed below.

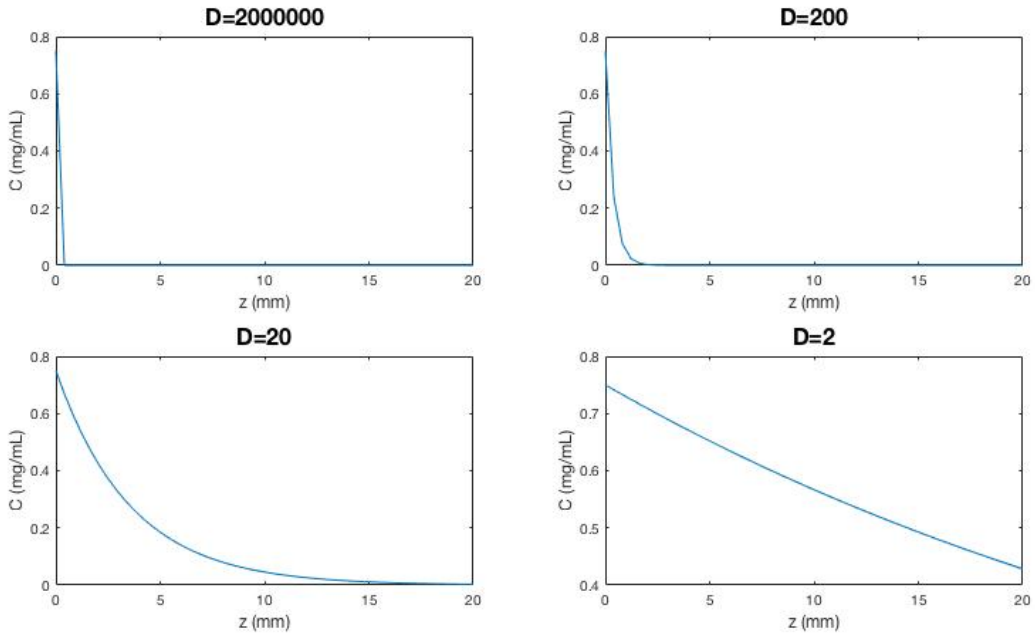

Figure 10: The concentration across the z-component of the blood vessel with different diffusivity constants.

As in case 1, changing the diffusion constant is the same as changing the mass transfer driving force. As the constant decreases, less urea is leaving the pipe (via the membrane), resulting in higher concentration at the blood vessel outlet. For cases where the diffusion constant is sufficiently large (D = 2000000, 200, 20 cm^2/s), the model predicts that the separation is achieved in 1 pass (which is not realistic. See Discussion section). For low diffusion, the logarithmic behavior is less pronounced and can be approximated with a linear function (similar to the mass transfer coefficient model).

Case 4

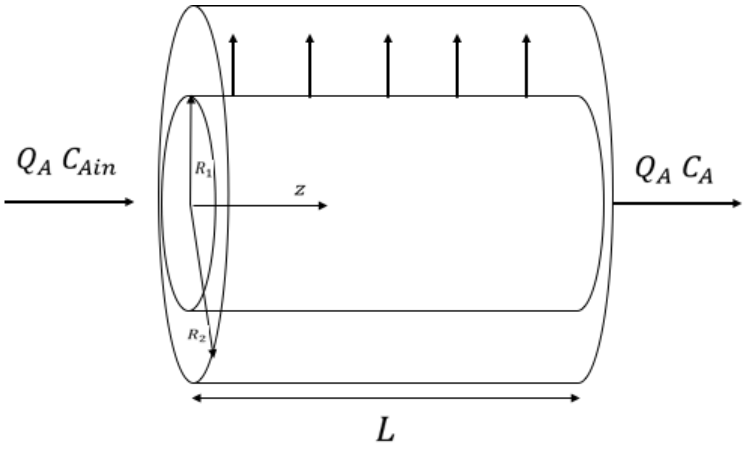

Figure 11: Model for the diffusion across the membrane across the length of the blood vessel

The concentration profile in the membrane across both the radial and z directions was also investigated. To do this, the profile along the inner wall was taken as the boundary condition for our diffusion equation at each z. The equation was then plotted along the radial direction.

As stated before, the solution to the diffusion equation was of the form:

$$\mathrm{C} = Aln(r) + B$$

$$A = \frac{-C(r = R_1)}{ln\left(\frac{R_2}{R_1}\right)}$$

$$B = \frac{C(r=R_1)}{ln\left(\frac{R_2}{R_1}\right)}\ln(R_2)$$

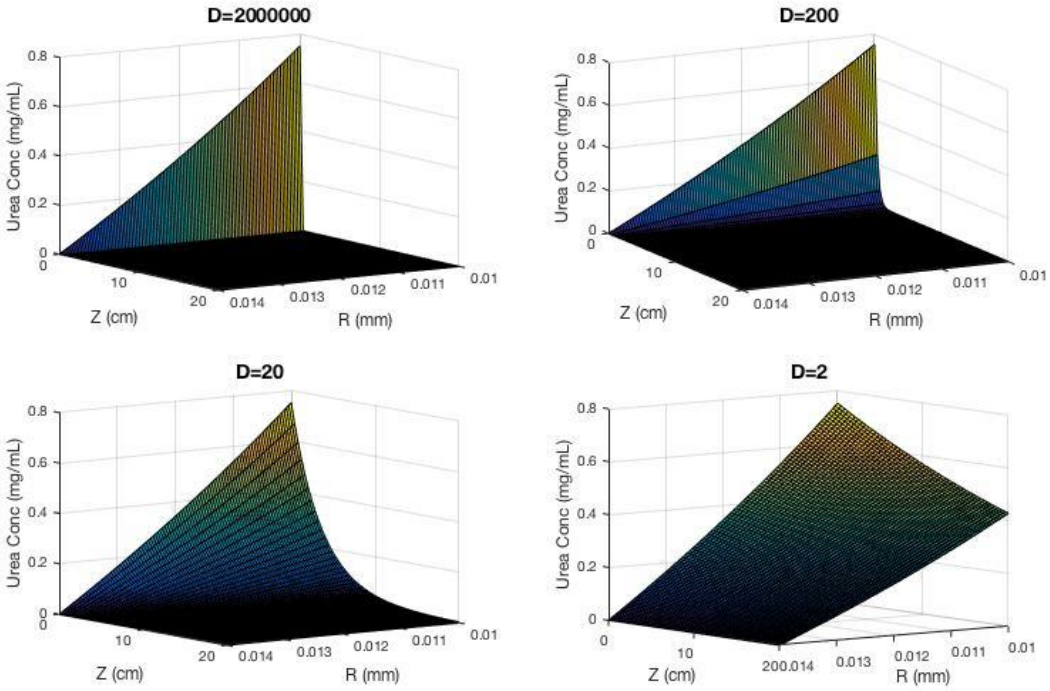

Figure 12: The concentration profile in the membrane in the radial and z-components with varying diffusivity constants

This membrane profile explains why the concentration profile in the blood vessel dropped so quickly. Virtually all of the urea diffusion occurs in the beginning of the membrane because of the high diffusivity constant, which leaves a minimal amount of urea left in the bloodstream. We also constructed graphs for lower diffusivity constants, which show a more gradual diffusion along the membrane, and a slower decay in concentration of urea in the blood stream.

Discussion

Model Limitations

There are multiple limitations to the models in cases 1 through 4. Beyond case 2, all cases were assumed to occur at steady state. Although this eventually will be true, we are neglecting start up behavior in the dialyzer. Additionally, we are assuming in every case that there is no change in volumetric flows in both the dialysate and blood flow. To make this assumption we are assuming a dilute concentration of urea in both flows. However, in true dialysis, both small molecule toxins and water are transferred through the membrane. Osmosis of water likely effects volumetric flows and this would impact mass transfer across the membrane. In addition, we neglected ultrafiltration as it would require inclusion of fluid flow equations affected by a pressure gradient across the membrane. If ultrafiltration were accounted for, faster mass transfer would be likely be observed as the pressure gradient would compound with the concentration gradient and provide additional driving force for the movement of urea across the membrane.

In cases 3 and 4 the results actually show that diffusion is not the main mode of transfer of urea across. As seen in Figure 12, only a low diffusion constant shows a reasonable concentration profile. This is because the model's assumption of only diffusion-driven transfer does not hold well. In reality, the urea would travel across the membrane as a result of both diffusion and convective flow. For dialysis in this case, convective flow transfer dominates and exhibits a behavior similar to that obtained when using mass transfer analysis. The model does show (for lower diffusivity constants) that diffusion would provide another source of resistance for mass transfer. In essence, if diffusion was a significant driving force, then the urea movement across the membrane would be even slower.

Together these assumptions account for the inaccuracy of the model, exhibited by the short time scale required to reach steady state in all of the cases when literature diffusion constants are used.

However, case 1 does not suffer from this problem as significantly because of how the mass transfer coefficient is defined. By simply lumping all of different driving forces together into one simple linear model, the model sacrifices the details of these driving forces for simplicity. The constant can be measured easily by simply determining the concentration of both compartments. The result is a less-detailed but more accurate model. The simplicity necessitates the need for a more complicated model if details such as the concentration gradient with respect to spatial dimensions are required. This was the motivation for cases 3 and 4.

Nevertheless, the presented models are useful in determining various design parameters. Varying parameters such as the mass transfer coefficient (case 1) and diffusion constant (cases 3 and 4) allow for *in silico* approximation for various membrane designs and even overall dialysis design. For instance, different membrane materials will strongly influence the diffusion across the membrane. This will change the steady state concentration and the total number of passes needed. These experiments would be tedious to run without such a model. Other factors that affect the diffusion include the porosity of the membrane and thickness of the membrane (cases 3 and 4). The volumetric flow rates of both compartments are also another important performance parameter. The higher the flow rate, the slower the concentration will change in both compartments (case 1). The studied models allow the designer to explore various parameters cheaply and quickly.

Next steps

While this study has proven useful in modeling dialysis, a few key components are missing to model the reality of the physical system especially when using equations that are determined from first principles like in cases 3 and 4. First, diffusion in the radial direction within the blood vessel was ignored because the diffusion should only significantly occur at the boundary due to blood flow. However, the radial dimension should be included to illustrate that velocity profile within the pipe is not truly uniform. For instance, in these conditions, laminar flow can be assumed due to the small diameter of the fibers, and a parabolic velocity profile can be fitted with the following equation:

$$V(r) = V_{max}(1 - ar^2)$$

where V_{max} is the maximum velocity (at the center of the tube), r is the radius of the pipe, and *a* is a tuning parameter. However, this detail was ignored for the derivation since including the radial dimension would have made the problem unsolvable by our available methods.

In order to account for convection, the volumes of both compartments should also be allowed to vary spatially and temporally to account for the movement of water across the membrane. This will increase the resistance of mass transfer of the system.

In addition, while the study only included a single tube, dialysis machines generally pack a bundle of tubes to increase the surface area to volume ratio. How the tubes are bundled will affect the overall diffusion. Hundreds of tubes can be simulated *in silico*. However, this problem poses additional challenges such as how to deal with the interface-interface diffusion between tubes and what the effects of the void space are on the diffusion (and whether the void space fluid will behave similarly to the bulk dialysate).

Finally, future studies can also investigate the effects of having additional toxins in the blood stream and how the mixture affects diffusion.

Conclusion

Through our results from each of our cases we have developed a comprehensive system for preliminary dialyzer design. In case 1 we created a bulk model which is useful for determining the number of passes through the dialyzer required to reduce blood toxin levels. In cases 1 and 2 we have demonstrated that we can use the bulk mass transfer model to observe membrane dynamics in spatial and temporal dimensions. We developed a model of diffusion across the semipermeable membrane over the length of the dialyzer in case 4. The combination of cases 1 through 4 are useful for determining the permeability (diffusivity) of the dialyzer membrane, and thus the membrane material, necessary to achieve the desired clearance of toxins from the bloodstream.

References

1. "Fast Facts." *The National Kidney Foundation*. N.p., 14 June 2016. Web. 2 Nov. 2016.
2. "UNC Kidney Center." *Glomerular Disease* -. N.p., n.d. Web. 2 Nov. 2016.
3. "Dialysis." *The National Kidney Foundation*. N.p., 16 Sept. 2016. Web. 2 Nov. 2016.
4. "How Hemodialysis Works." *Toltec International Inc*. N.p., 2006, Web. 2 Nov. 2016.
5. Katneni, Ratnaja. "Ratnaja Katneni MD, Nephrologist." *Ratnaja Katneni MD, Nephrologist*. N.p., n.d. Web. 2 Nov. 2016.
6. Cussler, E. L. *Diffusion: Mass Transfer in Fluid Systems*. Cambridge: Cambridge UP, 2009. Print.
7. Institute, Inc. Medical Education. "Lab Values Explained." *Kidney Disease Info*. N.p., n.d. Web. 11 Nov. 2016.
8. Cheung, Alfred. Ward, Richard. “Hemodialyzers.” *American Society of Nephrology. (2016)*

Supplement

Constants

All constants found in Reference 8.

Specification	Value
Blood Inlet Concentration	$75\,\frac{mg}{dl}$
Blood Flow Rate	$400\,\frac{ml}{min}$
Dialysate Flow Rate	$500\,\frac{ml}{min}$
Membrane Diameter	$40\,\mu mol$
Inner Diameter of Fibers	$200\,\mu mol$
Length of Fibers	$20\,cm$
Number of Fibers	$17{,}000$
Diffusivity of Urea in Cellulose Membrane	$2.7 * 10^{6}\,\frac{cm^2}{sec}$
Mass Transfer Area Coefficient of Urea in Cellulose Membrane	$700\,\frac{ml}{min}$

MatLab Code

Case 1

```
%Setting up Constants
r_tube = 100*1e-4; % cm
L_tube = 20; % cm

N = 17000; % Number of tubes

Vol_a = N*(pi*r_tube^2)*L_tube; %cm^2
Vol_b = 2000; % cm^2

v_a = 400/60; % mL/s
v_b = 500/60; % mL/s

Ca0 = 75/100; %mg/mL
Cb0 = 0;

k_list = [1400/60, 700/60, 100/60, 30/60]; %mL/s

for i = 1:size(k_list,2)
    k = k_list(i);

    %Solving for the Steady State solution
    M = [-(k + v_a), k; k, -(k + v_b)];
    gen = [-Ca0*v_a; -v_b*Cb0];

    steadySol = linsolve(M, gen);

    %Solving for the Homogeneous Solution
    [eigenVector, eigenValue] = eig(M);
    lambda1 = eigenValue(1,1);
    lambda2 = eigenValue(2,2);

    constants = linsolve(eigenVector, [Ca0; 0] - steadySol);

    a = eigenVector(1,1)*constants(1);
    b = eigenVector(2,1)*constants(1);
    c = eigenVector(1,2)*constants(2);
    d = eigenVector(2,2)*constants(2);

    e = steadySol(1);
    f = steadySol(2);

    t = 0:0.01:1;

    ca = a*exp(lambda1*t) + c*exp(lambda2*t) + e;
    cb = b*exp(lambda2*t) + d*exp(lambda2*t) + f;

    subplot(2,2,i)

    plot(t,ca,'b')
    hold on
```

```
    plot(t,cb,'--')
    ylim([0,0.75])

    % subplot(2,1,1);
    % plot(t,ca)
    % title('Concentration in the Tube')
    % ylabel('Time(mins)')
    %
    % subplot(2,1,2);
    % plot(t,cb)
    title(strcat('k = ', num2str(k*60), ' mL/min'))
    ylabel('Concentration (mg/mL)')
    xlabel('Time(mins)')

    % ylim([0,0.3])
end

legend('Blood Vessel', 'Dialysate')

Case 1 (Number of Passes)
n = 1;

%Setting up Constants
r_tube = 100*1e-4; % cm
L_tube = 20; % cm

N = 17000; % Number of tubes

Vol_a = N*(pi*r_tube^2)*L_tube; %cm^2
Vol_b = 2000; % cm^2

k = 700/60; %mL/s

v_a = 400/60; % mL/s
v_b = 500/60; % mL/s

Ca0 = 75/100; %mg/mL
Cb0 = 0;

k_list = [1400/60, 700/60, 100/60, 30/60];

for i = 1:size(k_list,2)
    k = k_list(i)
    n = 1;

    Ca0 = 75/100; %mg/mL
    Cb0 = 0;

    value = 1;

    concentration = zeros(1,1);
    concentration(1) = Ca0;
```

```
    while value >= 0.05
        %Solving for the Steady State solution
        M = [-(k + v_a), k; k, -(k + v_b)];
        gen = [-Ca0*v_a; -v_b*Cb0];

        steadySol = linsolve(M, gen);

        concentration(n + 1) = steadySol(1);

        Ca0 = steadySol(1);
        value = steadySol(1);

        n = n + 1;
    end

    subplot(2,2,i)
    bar(0:size(concentration,2) - 1, concentration)
    title(strcat('k = ', num2str(k*60), ' mL/min'))
    xlabel('Number of Passes')
    ylabel('Inlet Urea Concen (mg/mL)')
    xlim([-1,size(concentration,2)])
end
```

Case 2

```
m = 1;
R1=.1;
R2=.14;
r = linspace(R1,R2,50);
t = linspace(0,1);

sol = pdepe(m,@projectpde,@projectic,@projectbc,r,t);
u = sol(:,:,1);

surf(r(1:end),t(2:end),u(2:end,1:end))
xlabel('Distance(cm)')
ylabel('Time(s)')

figure
plot(t,u(:,1))

function [ c,f,s ] = projectpde( x,t,u,dudx )
D = 2.6E6;
c = 1/D;
f = dudx;
s = 0;
End

function [ u0 ] = projectic( x )
u0=[];
for i=1:length(x)
    if x(i) == 0
        u0(i)=.7481+.4337;
```

```
    else
        u0(i)=0;
    end
end
end

function [ pl,ql,pr,qr ] = projectbc( xl,ul,xr,ur,t )
pl=ul-(0.23*exp(-30.9*t)+.037*exp(-7.47*t)+.48);
ql=0;
pr=ur-(-.248*exp(-30.9*t)+.034*exp(-7.47*t)+.214);
qr=0;
end
```

Cases 3 and 4

```
clc
clear all

C0=.75;
z=linspace(0,20,50);
r=linspace(100E-4,140E-4);
v = 400/60/pi/(100E-4)^2;
R1 = 100E-4;
R2 = 140E-4;
D = [2E6,2E2,20,2];
for k=1:length(D)
   C1(k,:)=C0*exp(-D(k)/R1/log(R2/R1)/v*z);
end

%plot(z,C1(5,:))

C=[];

for i = 1:size(C1,1)
   for j = 1:size(C1,2)
      C(j,:)=C1(i,j)./log(R2/R1).*log(R2./r);
   end
   subplot(2,2,i)
   surf(r,z,C);
   xlabel('R (mm)')
   ylabel('Z (cm)')
   zlabel('Urea Conc (mg/mL)')
   title(strcat('D=', num2str((D(i)))))
%    figure
%    plot(z,C1)
end

%This is for the inner tube
% for i=1:size(C1,1)
%    subplot(2,2,i)
%    plot(z,C1(i,:))
%    xlabel('z (mm)')
%    ylabel('C (mg/mL)')
%    title(strcat('D=', num2str((D(i)))))
% end
```