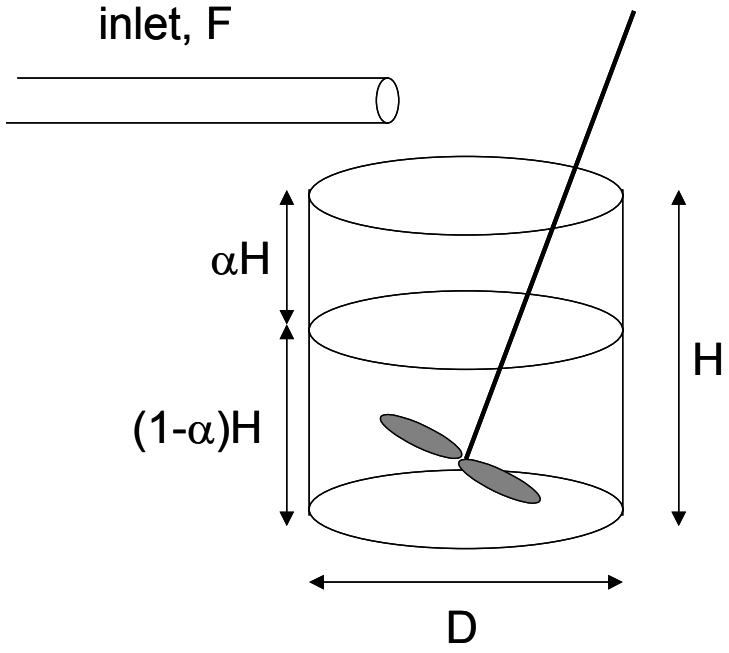
Midterm Examination
Administered: Thursday, December 5, 2002
SOLUTIONS

Problem (1)
In the undergraduate unit operations laboratory at the University of TN, (ChE 310), the students model a continuous stirred tank reactor that is stirred only partially creating a two-cell model. The reactor is run in overflow mode, meaning that the effluent simply pours out over the top of the tank.



The tank is cylindrical with height, H, and diameter, D. The two-cell model assumes that the concentration is homogeneous in each cell, but different between cells. α is the volume fraction of the top cell. The inlet volumetric flow rate is F, with concentration C_{in}.

Consider a binary system of salt dissolved in water. (Thus there is actually no chemical reaction in the 'reactor'.) Writing mole balances on salt for each volume yields

accumulation = in – out

$$\tau_1 \frac{dC_1}{dt} = -C_1(t) + \left(\frac{R}{R+F}\right)C_2(t) + \left(\frac{F}{R+F}\right)C_{in}$$

$$\tau_2 \frac{dC_2}{dt} = C_1(t) - C_2(t)$$

where C_1 is the concentration of salt in the top cell and C_2 is the concentration of salt in the bottom cell, τ_1 and τ_2 are the residence times for each cell, given by:

$$\tau_1 = \left(\frac{\alpha V}{R+F}\right) \quad \text{and} \quad \tau_2 = \left(\frac{(1-\alpha)V}{R}\right) \quad \text{where} \quad V = \frac{H\pi D^2}{4}$$

R is the volumetric exchange rate between the top and bottom cells.
Answer the following questions. Assume that R, F, H, D, C_{in} and α are not functions of time.

(a) We have a system of two ordinary differential equations. Are they linear or nonlinear?
(b) Is the system of ODEs homogeneous or non-homogeneous?
(c) Does this system of ODEs have an analytical solution? If so, what is the **general** form?
(d) What initial conditions need to be known to define a unique solution to this problem?
(e) Analytically calculate and report the eigenvalues of this system of equations.
(f) What is the critical point (steady state) of the system?
(g) Knowing that R, F, H, D and α are all real numbers strictly greater than zero, characterize the type of critical point as a proper/improper node, saddle point, center, or spiral point. Determine the stability of the critical point.
(h) Is there any combination of R, F, H, D and α that can change the type or stability of the critical point?

Solution:

(a) We have a system of two ordinary differential equations. Are they linear or nonlinear?

Both ODEs (and thus the system) are linear.

(b) Is the system of ODEs homogeneous or non-homogeneous?

The first ODE is non-homogeneous, meaning that the system must be treated as nonhomogeneous. (Actually if the inlet concentration is zero, then the problem is homogeneous.)

(c) Does this system of ODEs have an analytical solution? If so, what is the **general** form?

The solution of a system of linear non-homogeneous ODEs of the form

$$\frac{d\underline{y}}{dx} = \underline{\underline{A}}\,\underline{y} + \underline{b}(x) \tag{3.1}$$

$$\underline{y}(x = x_o) = \underline{y}_o \tag{3.2}$$

has the general form

$$\underline{y}_{nh}(x) = \underline{\underline{W}}_c \exp\left[\underline{\underline{\Lambda}}(x)\right] \left[\exp\left[\underline{\underline{\Lambda}}(x_o)\right]^{-1} \underline{\underline{W}}_c{}^{-1} \underline{y}_o - \underline{u}(x_o) + \underline{u}(x)\right] \tag{3.26}$$

where

$$\underline{u} = \int \exp\left[-\underline{\underline{\Lambda}}(x)\right] \underline{\underline{W}}_c{}^{-1} \underline{b}(x)\, dx \tag{3.23}$$

where $\underline{\underline{\Lambda}}$ is the matrix of eigenvalues and $\underline{\underline{W}}_c$ is the corresponding matrix of eigenvectors of $\underline{\underline{A}}$.

(d) What initial conditions need to be known to define a unique solution to this problem?

We need to know the concentration of each cell at time 0.

(e) Analytically calculate and report the eigenvalues of this system of equations.

If we rewrite our equations

$$\tau_1 \frac{dC_1}{dt} = -C_1(t) + \left(\frac{R}{R+F}\right)C_2(t) + \left(\frac{F}{R+F}\right)C_{in}$$

$$\tau_2 \frac{dC_2}{dt} = C_1(t) - C_2(t)$$

in the form of equation (3.1), we have for the $\underline{\underline{A}}$ matrix

$$\underline{\underline{A}} = \begin{bmatrix} -\frac{1}{\tau_1} & \frac{1}{\tau_1}\beta \\ \frac{1}{\tau_2} & -\frac{1}{\tau_2} \end{bmatrix} \quad \text{where} \quad \beta = \left(\frac{R}{R+F}\right)$$

The eigenvalues of this matrix are given by the characteristic equation, $\det\left(\underline{\underline{A}} - \lambda \underline{\underline{I}}\right) = 0$, which for this problem is a quadratic polynomial, yielding the eigenvalues as the two roots.

$$\left(-\frac{1}{\tau_1} - \lambda\right)\left(-\frac{1}{\tau_2} - \lambda\right) - \frac{1}{\tau_2}\frac{1}{\tau_1}\beta = \lambda^2 + \left(\frac{\tau_1 + \tau_2}{\tau_1\tau_2}\right)\lambda + \frac{1-\beta}{\tau_1\tau_2} = 0$$

Using the quadratic formula we have for the eigenvalues

$$\lambda = \frac{-\left(\frac{\tau_1 + \tau_2}{\tau_1\tau_2}\right) \pm \sqrt{\left(\frac{\tau_1 + \tau_2}{\tau_1\tau_2}\right)^2 - 4\frac{1-\beta}{\tau_1\tau_2}}}{2}$$

(f) What is the critical point (steady state) of the system?

The critical point occurs when the time derivatives are zero.

$$\begin{bmatrix} -\frac{1}{\tau_1} & \frac{1}{\tau_1}\beta \\ \frac{1}{\tau_2} & -\frac{1}{\tau_2} \end{bmatrix} \begin{bmatrix} C_{1,ss} \\ C_{2,ss} \end{bmatrix} = \begin{bmatrix} \frac{\beta - 1}{\tau_1} C_{in} \\ 0 \end{bmatrix}$$

Solving this system of two linear algebraic equations yields the critical point, which not surprisingly is $C_{1,ss} = C_{2,ss} = C_{in}$

(g) Knowing that R, F, H, D and α are all real numbers strictly greater than zero, characterize the type of critical point as a proper/improper node, saddle point, center, or spiral point. Determine the stability of the critical point.

We examine the eigenvalues. The only way that the critical point can be a spiral or a center is if the discriminant (the argument of the square root in the eigenvalue) is negative, yielding an imaginary component to the eigenvalue. Therefore, if we show that the discriminant is always positive, then we know we can eliminate a center and a spiral point.

Prove: $\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2 - 4\frac{1-\beta}{\tau_1\tau_2} > 0$

We recognize that $\tau_1 > 0$, $\tau_2 > 0$, and $0 < \beta < 1$.

$$(\tau_1+\tau_2)^2 - 4\tau_1\tau_2(1-\beta) > 0$$

$$\left(\tau_1{}^2 + 2\tau_1\tau_2 + \tau_2{}^2\right) - 4\tau_1\tau_2(1-\beta) > 0$$

In the worst case scenario, β approaches 0.

$$\left(\tau_1{}^2 + 2\tau_1\tau_2 + \tau_2{}^2\right) - 4\tau_1\tau_2 > 0$$

$$\left(\tau_1{}^2 - 2\tau_1\tau_2 + \tau_2{}^2\right) > 0$$

$$(\tau_1-\tau_2)^2 > 0$$

Since the residence times are real numbers, the square is positive, and the last statement is true by inspection. Thus the critical point is neither a center nor a spiral point. To distinguish between a node and a saddle point, we need to determine the signs of the (real) eigenvalues.

In order to determine the sign of the eigenvalues, we need to show that the square root term is smaller in magnitude than the magnitude of the term outside the square root, $\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)$.

This can be seen by inspection. β is less than one. Therefore, 1-β is positive. Thus $4\frac{1-\beta}{\tau_1\tau_2}$ is positive. Since we subtract this term, the argument inside the square root is always smaller than $\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2$. In the extreme case, β=1, and the term in the square root is equal to $\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2$. The square root of this term can be no larger than $\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)$. Thus the square root term is never larger in magnitude than the term outside the square root. As a result, the sign of the term outside the square root determines the signs of both of the eigenvalues. By inspection,

this term is negative. Both eigenvalues are negative. Therefore, this is an improper node. Moreover, because both eigenvalues are negative, the node is stable.

(h) Is there any combination of R, F, H, D and α that can change the type or stability of the critical point?

No. In part (g) we have provided a thorough proof, that all systems are stable, improper nodes.

NOT ASSIGNED IN THIS EXAM.
(i) Analytically determine the specific solution to this problem.

$$\begin{bmatrix} \frac{dC_1}{dt} \\ \frac{dC_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{1}{\tau_1} & \frac{1}{\tau_1}\beta \\ \frac{1}{\tau_2} & -\frac{1}{\tau_2} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} + \begin{bmatrix} \frac{1-\beta}{\tau_1} C_{in} \\ 0 \end{bmatrix}$$

In order to fill out the missing parts of equation (3.26)

$$\underline{y}_{nh}(x) = \underline{\underline{W}}_c \exp\left[\underline{\underline{\Lambda}}(x)\right] \left[\exp\left[\underline{\underline{\Lambda}}(x_o)\right]^{-1} \underline{\underline{W}}_c^{-1} \underline{y}_o - \underline{u}(x_o) + \underline{u}(x)\right] \qquad (3.26)$$

we require the eigenvalues and the eigenvectors.

The eigenvalues are from part (e)

$$\lambda_1 = \frac{-\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right) + \sqrt{\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2 - 4\frac{1-\beta}{\tau_1\tau_2}}}{2}$$

$$\lambda_2 = \frac{-\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right) - \sqrt{\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2 - 4\frac{1-\beta}{\tau_1\tau_2}}}{2}$$

We find the eigenvectors, $\underline{w}_i$, by solving $\left(\underline{\underline{A}} - \lambda_i \underline{\underline{I}}\right)\underline{w}_i = \underline{0}$ for i = 1 and 2. Performing this procedure yields the following eigenvectors:

$$\underline{w}_1 = \begin{bmatrix} \tau_2\lambda_1 + 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \underline{w}_2 = \begin{bmatrix} \tau_2\lambda_2 + 1 \\ 1 \end{bmatrix}$$

$$\underline{\underline{W}}_c = \begin{bmatrix} \underline{w}_1 & \underline{w}_2 \end{bmatrix} = \begin{bmatrix} \tau_2\lambda_1 + 1 & \tau_2\lambda_2 + 1 \\ 1 & 1 \end{bmatrix}$$

$$\det\left(\underline{\underline{W}}_c\right) = \tau_2\left(\lambda_1 - \lambda_2\right) = \tau_2\sqrt{\left(\frac{\tau_1+\tau_2}{\tau_1\tau_2}\right)^2 - 4\frac{1-\beta}{\tau_1\tau_2}}$$

$$\underline{\underline{W}}_c^{-1} = \frac{1}{\det\left(\underline{\underline{W}}_c\right)}\begin{bmatrix} 1 & -\tau_2\lambda_2 - 1 \\ -1 & \tau_2\lambda_1 + 1 \end{bmatrix}$$

All that remains is the determination of $\underline{u}(x)$.

$$\underline{u} = \int \exp\left[-\underline{\underline{\Lambda}}(x)\right] \underline{\underline{W}}_c^{-1}\underline{b}(x)\,dx \tag{3.23}$$

$$\underline{u} = \int\begin{bmatrix} \exp(-\lambda_1 x) & 0 \\ 0 & \exp(-\lambda_2 x) \end{bmatrix}\underline{\underline{W}}_c^{-1}\begin{bmatrix} \frac{1-\beta}{\tau_1}C_{in} \\ 0 \end{bmatrix} dx$$

$$\underline{u} = \frac{1}{\det\left(\underline{\underline{W}}_c\right)}\int \begin{bmatrix} \exp(-\lambda_1 x) & (-\tau_2\lambda_2 - 1)\exp(-\lambda_1 x) \\ -\exp(-\lambda_2 x) & (\tau_2\lambda_1 + 1)\exp(-\lambda_2 x) \end{bmatrix}\begin{bmatrix} \frac{1-\beta}{\tau_1}C_{in} \\ 0 \end{bmatrix} dx$$

$$\underline{u} = \frac{\frac{1-\beta}{\tau_1}C_{in}}{\det\left(\underline{\underline{W}}_c\right)}\int\begin{bmatrix} \exp(-\lambda_1 x) \\ -\exp(-\lambda_2 x) \end{bmatrix} dx$$

$$\underline{u} = \frac{\frac{1-\beta}{\tau_1}C_{in}}{\det\left(\underline{\underline{W}}_c\right)}\begin{bmatrix} -\frac{\exp(-\lambda_1 x)}{\lambda_1} \\ \frac{\exp(-\lambda_2 x)}{\lambda_2} \end{bmatrix}$$

The solution to the entire problem is obtained by substituting each term into equation (3.26).

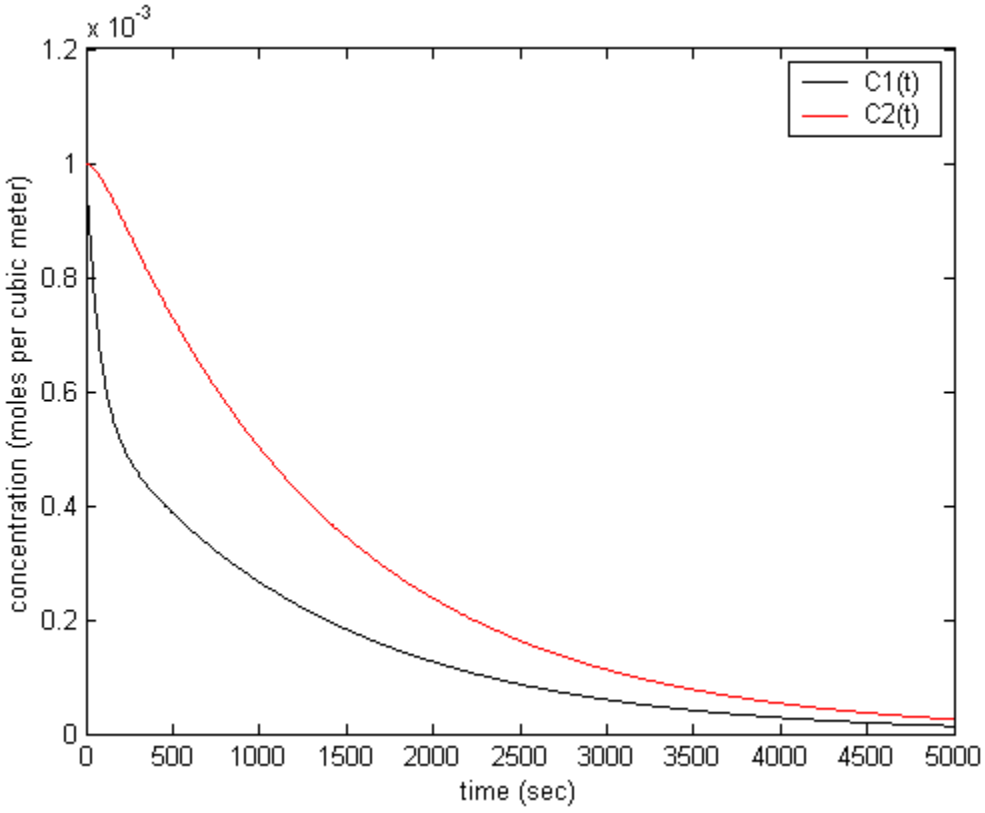
$$\underline{y}_{nh}(x) = \underline{\underline{W}}_c \exp\left[\underline{\underline{\Lambda}}(x)\right]\left[\exp\left[\underline{\underline{\Lambda}}(x_o)\right]^{-1}\underline{\underline{W}}_c^{-1}\underline{y}_o - \underline{u}(x_o) + \underline{u}(x)\right] \tag{3.26}$$

$$\underline{C}(x) = \frac{1}{\det\left(\underline{\underline{W}}_c\right)} \begin{bmatrix} \tau_2\lambda_1 + 1 & \tau_2\lambda_2 + 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \exp(\lambda_1 x) & 0 \\ 0 & \exp(\lambda_2 x) \end{bmatrix}$$

$$\left\{ \begin{bmatrix} \exp(-\lambda_1 x_o) & 0 \\ 0 & \exp(-\lambda_2 x_o) \end{bmatrix} \begin{bmatrix} 1 & -\tau_2\lambda_2 - 1 \\ -1 & \tau_2\lambda_1 + 1 \end{bmatrix} \begin{bmatrix} C_{1,o} \\ C_{2,o} \end{bmatrix} + \frac{1-\beta}{\tau_1} C_{in} \begin{bmatrix} -\dfrac{\exp(-\lambda_1 x) - \exp(-\lambda_1 x_o)}{\lambda_1} \\ \dfrac{\exp(-\lambda_2 x) - \exp(-\lambda_2 x_o)}{\lambda_2} \end{bmatrix} \right\}$$

Here is a plot of the solution for the following parameters:

Height of tank (m)	H = 1
Diameter of tank (m)	D = 1
volume fraction of top cell	alpha = 0.2
Inlet Flow rate (m^3/sec)	F = 1.e-3
Cell Exchange Flow rate (m^3/sec)	R = 1.e-3
inlet concentration (moles/m^3)	Cin = 0.0
INITIAL CONDITIONS	
initial time (sec)	to = 0
initial concentrations (moles/m^3)	co(1) = 1.0e-3
	co(2) = 1.0e-3



Here is the code I used to generate the plot.

```
%
%  ChE 505  Exam 2
%  Fall 2002
%  Author:  David Keffer
%
clear all;
close all;
format long;
%
%  INPUTS
%
% Height of tank (m)
H = 1;
% Diameter of tank (m)
D = 1;
% volume fraction of top cell
alpha = 0.2;
% Inlet Flowrate (m^3/sec)
F = 1.e-3;
% Cell Exchange Flowrate (m^3/sec)
R = 1.e-3;
% inlet concentration (moles/m^3)
Cin = 0.0000;

%
%  INITIAL CONDITIONS
%
% initial time (sec)
to = 0;
% co = initial concentrations (moles/m^3)
co = zeros(2,1);
co(1) = 1.0e-3;
co(2) = 1.0e-3;

%
%  Discretize time
%
% final time (sec)
tf = 5000;
% number of intervals
nint = 1000;

%
% CALCULATED TERMS
%
% reactor volume
V = H*pi*(D/2)^2;
% residence times
tau1 = alpha*V/(R+F);
tau2 = (1-alpha)*V/R;
% beta
beta = R/(R+F);
% discriminant
b = (tau1 + tau2)/(tau1*tau2);
discrim = b^2 - 4*(1-beta)/(tau1*tau2)
% eigenvalues
lambda = zeros(2,1);
lambda(1) = 0.5*(-b + sqrt(discrim) );
lambda(2) = 0.5*(-b - sqrt(discrim) );
lambda
% eigenvectors
Wc = zeros(2,2);
Wc(1,1) = tau2*lambda(1) + 1;
Wc(2,1) = 1;
Wc(1,2) = tau2*lambda(2) + 1;
Wc(2,2) = 1;
Wc
% determinant of Wc
detWc = tau2*sqrt(discrim);
%inverse of Wc
invWc = zeros(2,2);
invWc(1,1) = Wc(2,2);
invWc(2,2) = Wc(1,1);
invWc(1,2) = -Wc(1,2);
invWc(2,1) = -Wc(2,1);
invWc = 1/detWc*invWc;
invWc
% inverse of exponential of lambda at to
ielto = zeros(2,2);
ielto(1,1) = exp(-lambda(1)*to);
ielto(2,2) = exp(-lambda(2)*to);
% u at to
uo = zeros(2,1);
ufac = (1-beta)/(tau1*detWc)*Cin;
uo(1) = -ufac*exp(-lambda(1)*to)/lambda(1);
uo(2) = ufac*exp(-lambda(2)*to)/lambda(2);

%
% discretize time
%
dt = (tf-to)/nint;
np = nint + 1;
tvec = [to:dt:tf];

%
% evaluate solution at each time and store in cvec
%
cvec = zeros(2,np);
for i = 1:1:np
   t = tvec(i);
   u = zeros(2,1);
   u(1) = -ufac*exp(-lambda(1)*t)/lambda(1);
   u(2) =  ufac*exp(-lambda(2)*t)/lambda(2);
   elt = zeros(2,2);
   elt(1,1) = exp(lambda(1)*t);
   elt(2,2) = exp(lambda(2)*t);
   cvec(1:2,i) = Wc*elt*(ielto*invWc*co - uo + u);
end

% plot solution
figure(1);
plot(tvec,cvec(1,:),'k-');
hold on;
plot(tvec,cvec(2,:),'r-');
hold off;
xlabel('time (sec)');
ylabel('concentration (moles per cubic meter)');
legend('C1(t)','C2(t)');
```

Problem (2)

In problem (1), the two-cell model was used because a one-cell model failed to describe the experimental behavior of the poorly mixed reactor properly. Perhaps, the two-cell model described in problem (1) is also inadequate. One could increase the number of cells and create a three-cell model or a four-cell model, to allow finer gradations in the concentration as a function of axial position in the tank. Extending this idea, one could create a model with an infinite number of cells. In this model, each cell has the same fraction of volume, α, which is infinitesimally small.

(a) Write out the material balance(s) for the infinite-cell model.
(b) What kind of equation do you have: AE, ODE, PDE, or IE?
(c) Is the resulting equation linear or nonlinear?
(d) What initial and boundary conditions do you need?
(e) Describe in adequate detail the numerical algorithm that you would use to solve the problem. Discuss in particular any problems that you foresee.
(f) In the two-cell model, R is a single number. Discuss the new form of R in the infinite-cell model.

Solution:

(a) Write out the material balance(s) for the infinite-cell model.

In the infinite-cell model, the concentration becomes a continuous function of axial height. So, instead of writing an ODE for the concentration in each cell, we now write a PDE for the reactor concentration. Each cell is now accounted for in the new spatial-dimensionality of the concentration.

The volumetric exchange rate, R, listed above is not a convection term since the exchange is both ways, resulting in no net flow. Instead this R is now manifested as a "diffusion term" or more accurately in this scenario a "dispersion term", where R must now have units of diffusivity, or square meters per time, rather than cubic meters per time. Let's perform a shell balance on one of the cells of width Δz.

$$V = A_{cross}\Delta z = \pi\left(\frac{D}{2}\right)^2 \Delta z$$

accumulation = in – out + generation

$$V\frac{\partial C(t,z)}{\partial t} = A_{cross}q(t,z)\Big|_z - A_{cross}\,q(t,z)\Big|_{z+\Delta z} + 0$$

where q is the dispersive flux. Divide by V and take the limit as Δz. approaches 0.

$$\frac{\partial C(t,z)}{\partial t} = -\frac{\partial[q(z)]}{\partial z}$$

We assume that we can write a Fickian-like flux statement for q

$$q = -R\frac{\partial[C(t,z)]}{\partial z}$$

$$\frac{\partial C(t,z)}{\partial t} = \frac{\partial}{\partial z}\left(R(z)\frac{\partial[C(t,z)]}{\partial z}\right)$$

If R is independent of z then we can pull it out of the derivative.

(b) What kind of equation do you have: AE, ODE, PDE, or IE?

The equation is a parabolic PDE, because the unknown, C, is a function of both space and time. It is parabolic because the highest order time derivative is 1.

(c) Is the resulting equation linear or nonlinear?

The equation is linear in the unknown, i.e. concentration.

(d) What initial and boundary conditions do you need?

We need to know the concentration in the tank at the initial time at all axial positions.

$$C(t = t_o, z) = C_o(z)$$

At z=H (the bottom of the tank), we know that there is no mass flux. Therefore we have a Neumann boundary condition.

$$\left.\frac{\partial C(t,z)}{\partial z}\right|_{z=H} = 0$$

At z=0 (the top of the tank), we need a boundary condition that accounts for the concentration of the inlet flow. If we use a Dirichlet boundary condition, then we have the following condition:

$$C(t, z = 0) = C_{in}(t)$$

The puzzling thing about this choice of boundary condition is that our system is no longer a function of F, the inlet flow rate. Therefore, one would guess that this is an unphysical boundary condition. Moreover, this boundary condition would indicate that the effluent is always of concentration C_{in}.

Alternatively at this boundary node, we could write the following balance over the salt in the *entire tank*:

$$V\frac{\partial C_{TANK}(t)}{\partial t} = FC_{in} - FC(t, z = 0)$$

We have two unknowns here, $\frac{\partial C_{TANK}(t)}{\partial t}$ and $C(t, z = 0)$. However,

$$\frac{\partial C_{TANK}(t)}{\partial t} = \frac{1}{L}\frac{\partial}{\partial t}\int_{z=0}^{z=L} C(t,z)dz = \frac{1}{L}\int_{z=0}^{z=L}\frac{\partial C(t,z)}{\partial t}dz = \frac{1}{L}\int_{z=0}^{z=L}\frac{\partial}{\partial z}\left(R(z)\frac{\partial[C(t,z)]}{\partial z}\right)dz$$

$$\frac{\partial C_{TANK}(t)}{\partial t} = \frac{1}{L}\left\{\left[R(z)\frac{\partial[C(t,z)]}{\partial z}\right]_{z=L} - \left[R(z)\frac{\partial[C(t,z)]}{\partial z}\right]_{z=0}\right\}$$

Remember that at our lower boundary condition, the flux is zero.

$$\frac{\partial C_{TANK}(t)}{\partial t} = \frac{1}{L}\left\{0 - \left[R(z)\frac{\partial[C(t,z)]}{\partial z}\right]_{z=0}\right\}$$

Plugging this back into our balance over the tank, we have

$$-\frac{V}{L}\left[R(z)\frac{\partial[C(t,z)]}{\partial z}\right]_{z=0} = FC_{in} - FC(t,z=0)$$

This is a mixed boundary condition. We can use the same technique that we use to implement Neumann boundary conditions, to implement the mixed boundary condition.

(e) Describe in adequate detail the numerical algorithm that you would use to solve the problem. Discuss in particular any problems that you foresee.

This is a simple PDE to solve, assuming we know R(z). The easiest thing to do is assume that R is not a function of axial position within the tank. Then we simply can fit the equation for the right value of R.

Assuming we know R, we solve this using a Crank-Nicholson method. We choose Crank-Nicholson because the equation is linear, and the Crank-Nicholson method has the advantage over other second-order methods (like the second-order Runge-Kutta method) or taking advantage of the linearity of the PDE.

(f) In the two-cell model, R is a single number. Discuss the new form of R in the infinite-cell model.

As we said before, in this new model, R is a dispersion coefficient, which has the same units as diffusivity. It is still a measure of the effective exchange rate between adjacent cells.