Name: Robert Heeter

EXAM 3 - BIOE 391
Take Home – 2022

This portion of the exam is **open book/open notes**. Any other resources used must be acknowledged. Please **READ ALL INSTRUCTIONS**, manage your time effectively and answer the questions concisely but completely. Please upload a hard copy of the exam as a single PDF or Word file to Canvas. Handwritten formulas (equations) and diagrams are OK if the files are clearly scanned. Please make sure your file is clearly readable before uploading it. The recommended time investment in this take-home exam should be of no more than **5 hours**, although you are allowed to use more.

On my honor, I have neither given nor received any unauthorized aid on this exam.

Signature: Robert Heeter

Read Carefully!

Please comment your code as much as possible. This will help us to grade and give YOU partial credit.

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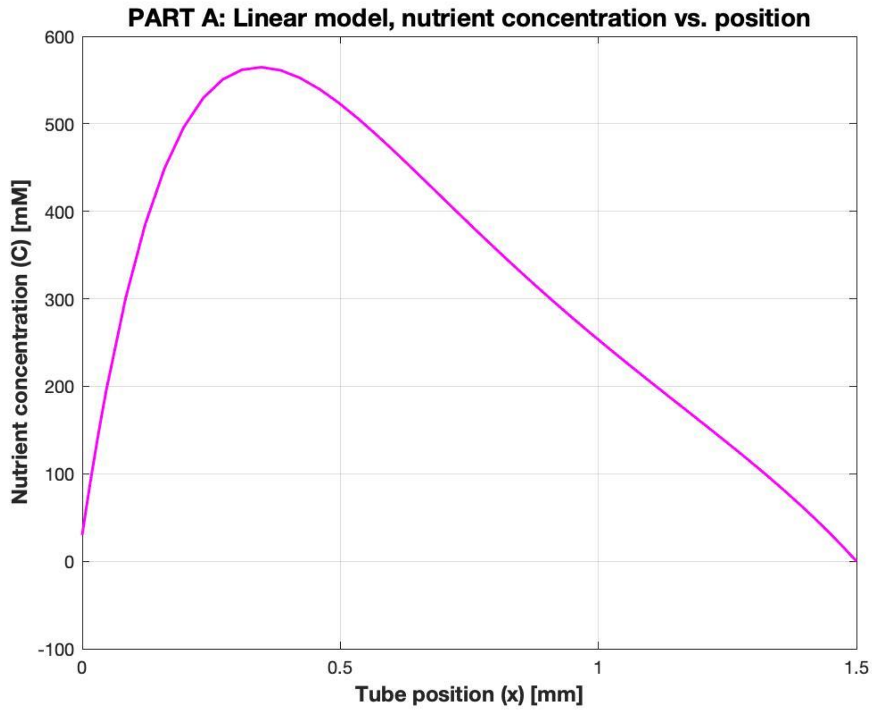
BIOE 391 Numerical Methods – Due 3 May 2022

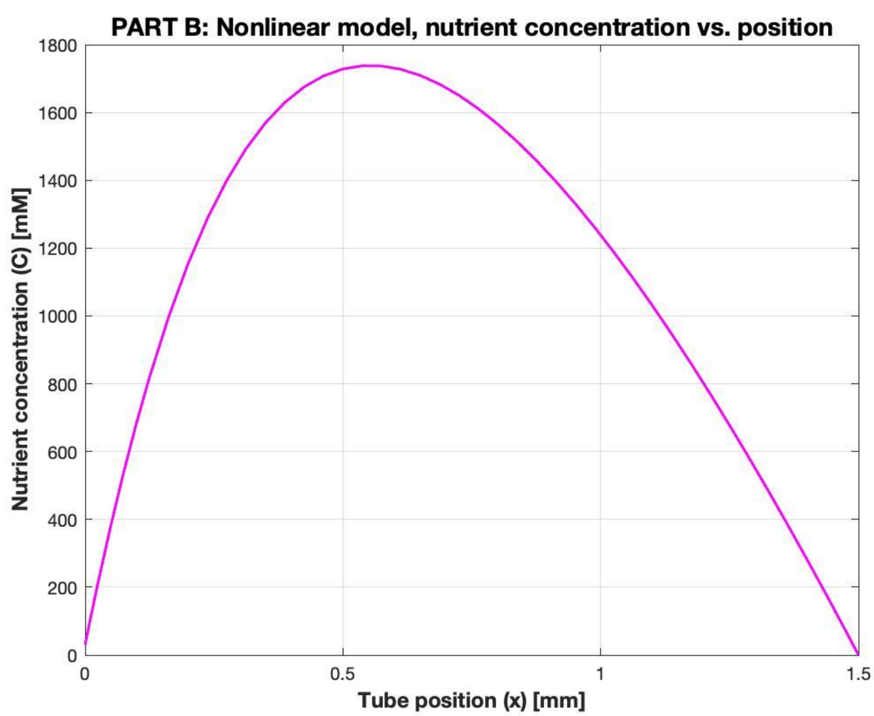
Exam 3 Solutions

1.

a. Figure *(also see end of document for handwritten work)*



b. Figure *(also see end of document for handwritten work)*



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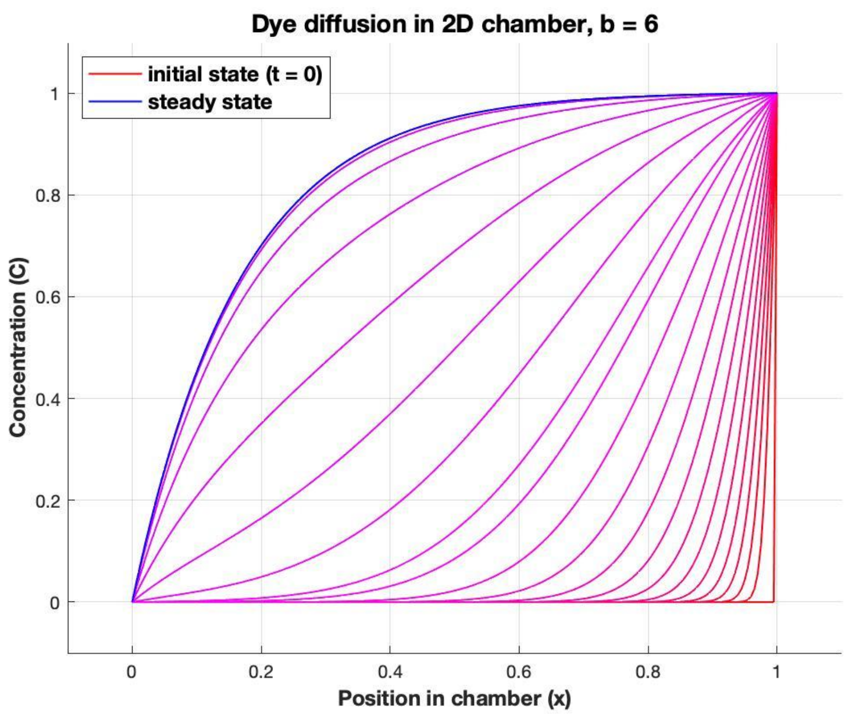
2.

- **a.** *See end of document for handwritten work and MATLAB code below.*
- **b.** *See MATLAB code below.*
- **c.** *See MATLAB code below.*
- **d.** **Figure** (*b = 6*)



e. **Figure** (*b = –4*)

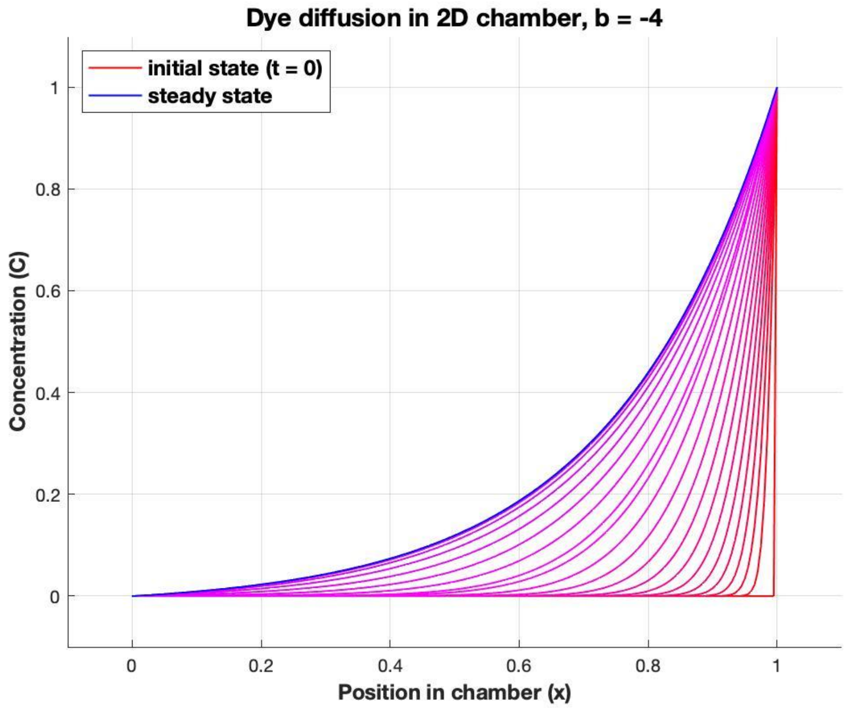


Figure (*b = –2*)

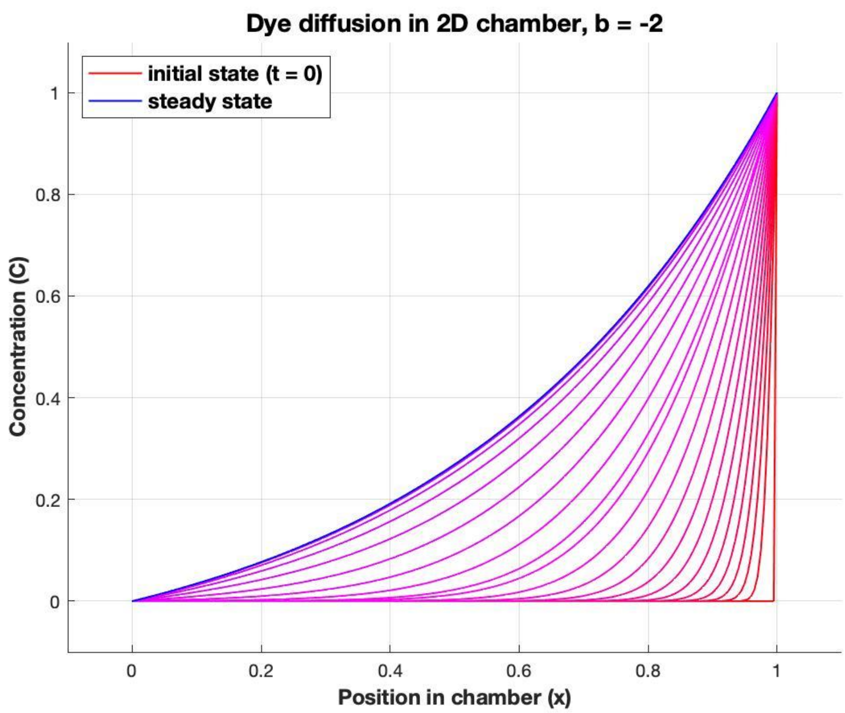


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Figure (*b = 0*)

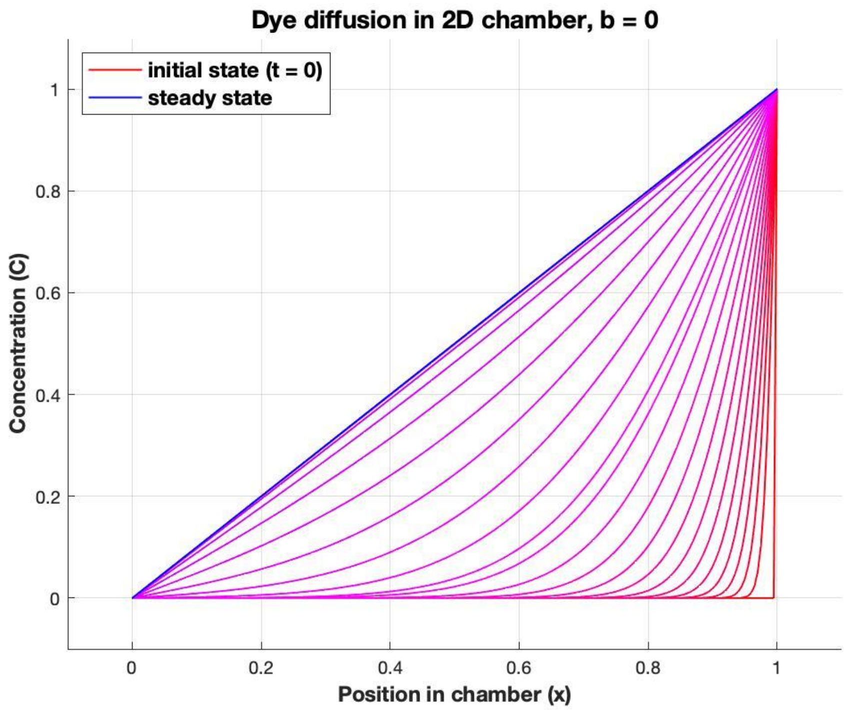


Figure (*b = 2*)

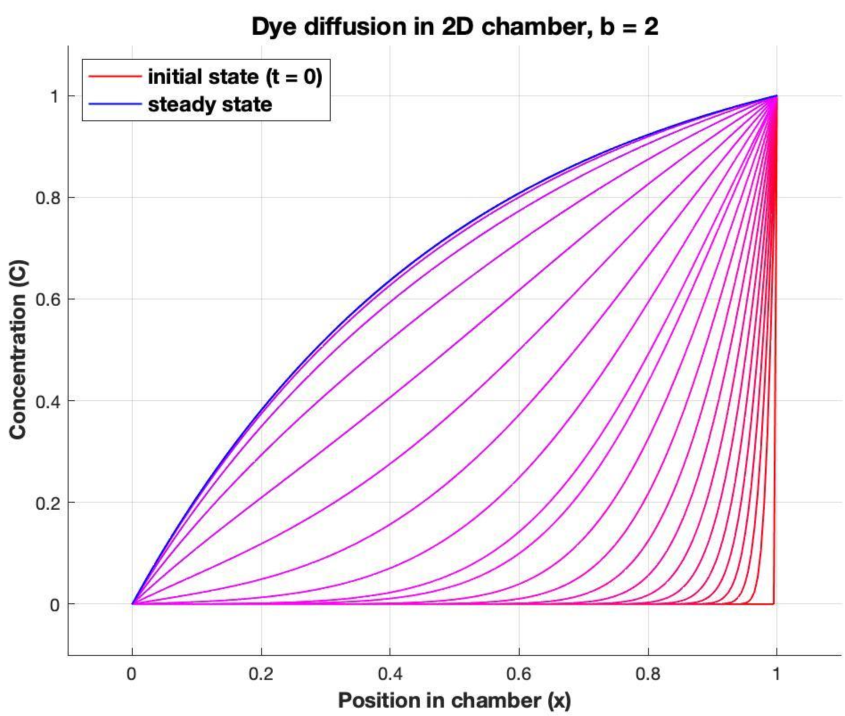
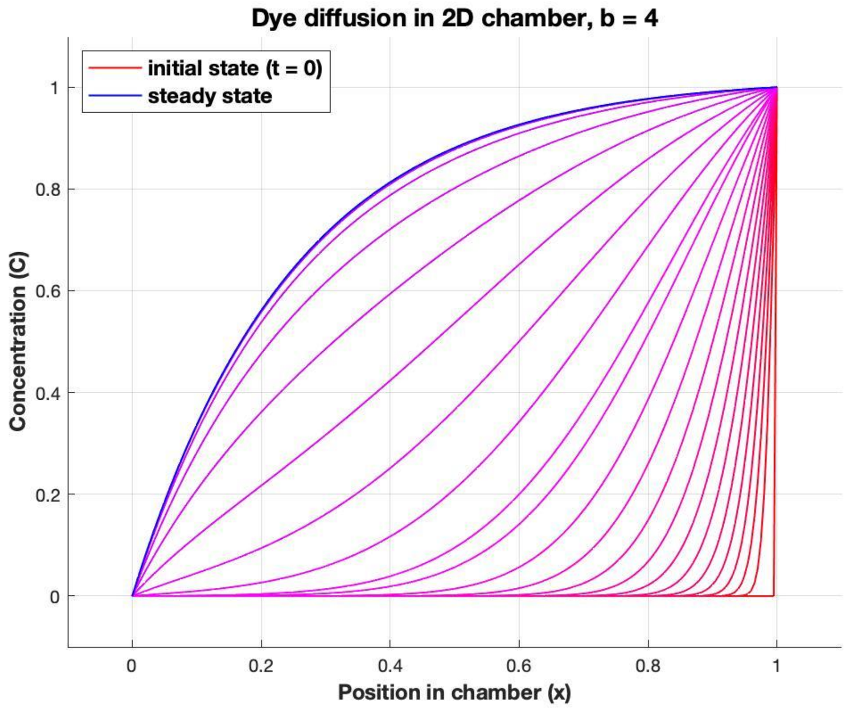


Figure (*b = 4*)



f. Bonus

The dispersion term, *b*, affects the steady-state solution of the system (blue line on the graphs in part E). When $b > 0$, the steady-state solution bows outward, meaning the dye maintains a higher concentration as it diffuses from the source at $x = 1$ to the sink at $x = 0$ in the chamber. When $b = 0$, the steady-state solution is a linear relationship between position and concentration. When $b < 0$, the steady-state solution bows inward, meaning the dye drops in concentration and has a lower concentration as it diffuses from $x = 1$ to $x = 0$. For any value of *b*, the system starts in the same initial state (red line on the graphs in part E), but over time the concentration spread of the dye shifts according to the dispersion term.

1. a. $D \frac{d^2C}{dx^2} - kC + F \frac{1}{x^2+x_0^2} = 0$

set $z = \frac{dC}{dx}$

$\frac{dz}{dx} = \frac{d^2C}{dx^2} \longrightarrow \frac{dz}{dx} = \frac{1}{D}\left(kC - F \frac{1}{x^2+x_0^2}\right)$

$\therefore \begin{cases} \frac{dC}{dx} = z \\ \frac{dz}{dx} = \frac{1}{D}\left(kC - F \frac{1}{x^2+x_0^2}\right) \end{cases}$

b. $D \frac{d^2C}{dx^2} - \frac{kC}{1+C/K_m} + F \frac{1}{x^2+x_0^2} = 0$

set $z = \frac{dC}{dx}$

$\frac{dz}{dx} = \frac{d^2C}{dx^2} \longrightarrow \frac{dz}{dx} = \frac{1}{D}\left(\frac{kC}{1+C/K_m} - F \frac{1}{x^2+x_0^2}\right)$

$\therefore \begin{cases} \frac{dC}{dx} = z \\ \frac{dz}{dx} = \frac{1}{D}\left(\frac{kC}{1+C/K_m} - F \frac{1}{x^2+x_0^2}\right) \end{cases}$

2a. PDE: $\frac{\partial^2 c}{\partial x^2} + b\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t}$

★ Second-order finite difference (Crank formulation):

① $\frac{\partial^2 c}{\partial x^2} = \frac{1}{2}\left[\frac{C_{i+1,n+1} - 2C_{i,n+1} + C_{i-1,n+1}}{\Delta x^2} + \frac{C_{i+1,n} - 2C_{i,n} + C_{i-1,n}}{\Delta x^2}\right]$

② $\frac{\partial c}{\partial t} = \frac{C_{i,n+1} - C_{i,n}}{\Delta t}$

③ $\frac{\partial c}{\partial x} = (b)\left(\frac{1}{2}\right)\left[\frac{C_{i+1,n+1} - C_{i-1,n+1}}{2\Delta x} + \frac{C_{i+1,n} - C_{i-1,n}}{2\Delta x}\right]$

Combine ①②③ into PDE to give: = coef matrix of coefficients

[Interior equations]:

$$\left(\frac{1}{2\Delta x^2} - \frac{b}{4\Delta x}\right) C_{i-1,n+1} + \left(-\frac{1}{\Delta x^2} - \frac{1}{\Delta t}\right) C_{i,n+1} + \left(\frac{1}{2\Delta x^2} + \frac{b}{4\Delta x}\right) C_{i+1,n+1} \ldots$$

$$\ldots = \underbrace{\left(-\frac{1}{2\Delta x^2} + \frac{b}{4\Delta x}\right) C_{i-1,n} + \left(\frac{1}{\Delta x^2} - \frac{1}{\Delta t}\right) C_{i,n} + \left(-\frac{1}{2\Delta x^2} - \frac{b}{4\Delta x}\right) C_{i+1,n}}_{= d \text{ vector}}$$

[Initial equation]: $C_{1,1} = 0$

[End equation]: $C_{end,\, end} = 1$

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Complete MATLAB Code

```
% Robert Heeter
% BIOE 391 Numerical Methods
% EXAM 3 MATLAB SCRIPT

clc, clf, clear, close all

%% PROBLEM 1, PART A
disp('PROBLEM 1A');

xint = [0 1.5]; % tube length (mm)
Ci = 30; % boundary conditions
Cf = 0;

z1 = 10; % guess z value for first two shots
z2 = 50;

[~,y1] = ode45(@linearrd,xint,[Ci z1]); % first shot
[~,y2] = ode45(@linearrd,xint,[Ci z2]); % second shot

za = z1 + (((z2-z1)/(y2(end,1)-y1(end,1)))*(Cf-y1(end,1))); % linear regression
[x3,y3] = ode45(@linearrd,xint,[Ci za]); % final shot

figure % plot results
plot(x3,y3(:,1),'-m','LineWidth',1.5)
xlabel('Tube position (x) [mm]','FontSize',12,'FontWeight','bold');
ylabel('Nutrient concentration (C) [mM]','FontSize',12,'FontWeight','bold');
title('PART A: Linear model, nutrient concentration vs. position','FontSize',14,'FontWeight','bold');
grid on


%% PROBLEM 1, PART B
disp('PROBLEM 1B');

xint = [0 1.5]; % tube length (mm)
Ci = 30; % boundary conditionsc

zguess = 0; % initial guess value for za
[za,r] = fzero(@res,zguess); % minimize z to fit boundary condition with fzero using res function below
[x,y] = ode45(@nonlinearrd,xint,[Ci za]); % final shot

figure % plot results
plot(x,y(:,1),'-m','LineWidth',1.5)
xlabel('Tube position (x) [mm]','FontSize',12,'FontWeight','bold');
ylabel('Nutrient concentration (C) [mM]','FontSize',12,'FontWeight','bold');
title('PART B: Nonlinear model, nutrient concentration vs.
position','FontSize',14,'FontWeight','bold');
grid on


%% PROBLEM 2, PART A-D
disp('PROBLEM 2A-D');

% PART A-C: b = 6
b = 6; % dispersion term
dyediffusion(b); % use dyediffusion function below to solve and graph

% PART E: b = -4,-2,0,2,4
for b = -4:2:4
    dyediffusion(b);
end


%% PROBLEM 2, PART E
```

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```
disp('PROBLEM 2E');

% No code necessary; see solution document


%% Additional Functions

function dy = linearrd(x,y)
% ABOUT: Linear system of ODEs to model the reaction and diffusion of
% nutrient in a chamber.

F = 0.8; % influx constant (mM/s)
x0 = 0.4; % influx constant (mm)
k = 3e-3; % consumption constant (1/s)
D = 2.5e-4; % diffusion constant (mm^2/s)

dy = [y(2);(1/D)*((k*y(1))-(F*(1/(x^2+x0^2))))]; % system

end


function dy = nonlinearrd(x,y)
% ABOUT: Nonlinear system of ODEs to model the reaction and diffusion of
% nutrient in a chamber.

F = 0.8; % influx constant (mM/s)
x0 = 0.4; % influx constant (mm)
k = 3e-3; % consumption constant (1/s)
D = 2.5e-4; % diffusion constant (mm^2/s)
KM = 2.5; % reaction constant (mM)

dy = [y(2);(1/D)*((k*y(1)/(1+(y(1)/KM)))-(F*(1/(x^2+x0^2))))]; % system

end


function r = res(za)
% ABOUT: Determines residual of nonlinear ODE at boundary for a given input
% za initial guess.

xint = [0 1.5]; % tube length (mm)
Ci = 30; % boundary conditions
Cf = 0;

[~,y] = ode45(@nonlinearrd,xint,[Ci,za]); % shot
r = y(end,1)-Cf; % residual

end


function [] = dyediffusion(b)
% ABOUT: Crank-Nicolson formulation to solve dye diffusion PDE with
% dispersion term b.

% Total number of nodes (chosen for good accuracy)
imax=201; % spatial index
nmax=200; % time index

% Initial step sizes
dx = 1/(imax-1);
dt = dx^2;

% Preallocate concentration matrix
C = zeros(imax,nmax+1);

% Initial conditions
```

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```
C(:,1) = 0; % C(x,0) = 0
x = (0:dx:1)'; % space vector
t = 0; % time = 0

% Dirichlet boundary conditions
C(1,:) = 0; % C(0,t) = 0
C(end,:) = 1; % C(1,t) = 1

% Iterate for each time step
for n = 1:nmax

    % Dirichlet boundary conditions
    C(1,n+1) = 1;
    C(end,n+1) = 1;

    % Set values for tridiagonal matrix coef for coef*C(:,n+1)=d
    coef = zeros(imax,imax); % C(~,n+1)
    dim = size(coef);

    diag_mid = 1:(dim(1)+1):(dim(1)*dim(2)); % indices for middle diagonal
    diag_up = dim(1)+1:(dim(1)+1):(dim(1)*dim(2)); % indices for upper diagonal
    diag_low = 2:(dim(1)+1):(dim(1)*dim(2)); % indices for lower diagonal

    coef(diag_mid) = (-1/(dx^2)) + (-1/dt); % C(i,n+1)
    coef(diag_up) = (1/(2*dx^2)) + (b/(4*dx)); % C(i+1,n+1)
    coef(diag_low) = (1/(2*dx^2)) + (-b/(4*dx)); % C(i-1,n+1)

    coef(1,1:2) = [1,0]; % following Dirichlet boundary conditions
    coef(end,end-1:end) = [0,1];

    % Set values for d vector
    d = zeros(imax,1); % d(i-1/i/i+1,n)

    d1 = ((-1/(2*dx^2))+(b/(4*dx))) * C((1:end-2),n); % terms for d vector
    d2 = ((1/(dx^2))+(-1/dt)) * C((2:end-1),n);
    d3 = ((-1/(2*dx^2))+(-b/(4*dx))) * C((3:end),n);
    d(2:end-1) = d1+d2+d3;

    d(1) = 0; % following Dirichlet boundary conditions
    d(end) = 1;

    % Solve system using backslash and update concentration matrix
    C(:,n+1) = coef\d;

    % Update time and increase delta t by 10% each step
    t = t+dt;
    dt = 1.1*dt;

end

% Plot C vs. x for various values of t
figure
hold on
for i = 1:4:nmax/4
    plot(x,C(:,i),'Color',[1,0,0+(i/(nmax/4))],'LineWidth',1);
end
for i = (nmax/4)+1:4:nmax
    plot(x,C(:,i),'Color',[1-((i-(nmax/4))/(3*nmax/4)),0,1],'LineWidth',1);
end
title(['Dye diffusion in 2D chamber, b = ', num2str(b)],'FontSize',14','FontWeight','bold');
xlabel('Position in chamber (x)','FontSize',12,'FontWeight','bold');
ylabel('Concentration (C)','FontSize',12,'FontWeight','bold');
legend('initial state (t =
0)','','','','','','','','','','','','','','','','','','','','','','','','','','','','','','','','','','',
'','','','','','','','','','','','','','','','','steady
state','FontSize',12,'FontWeight','bold','Location','northwest')
```

```
axis([-0.1,1.1,-0.1,1.1]);
hold off
grid on

end
```