%This code is used to simulate fluo evolution over time for a given initial AHL amount.

%Mathematical model:

% Variables: S: AHL; F: Fluorescence; N: cell density

% dS/dt = Diff\_s \* d^2/dx^2 (S) - gamma\_s \* S ;

% dF/dt = afa\_f \* N \* S/(K\_s + S) - gmma\_f \* F ;

% dN/dt = afa\_n \* N \* (1 - N/N\_l);

clear all;

close all;

% There are two ways to normalize:

% Divide everything by the mean fluo at T=0;

% Minus everything by the mean fluo at T=0;

subfold = 202 ; %202 or 503;

timeidi = 31;

timeidf = timeidi + 3;

%Load pamameters;

%===============================================

%========== Original parameters ====================

% gamma\_f = 0.04;

% gamma\_n = 0.00;

% beta\_f = 0.0;

% K\_s = 3.0e0; %uM

% N\_l = 5.0;

%========== new parameters for 503 ====================

if (subfold == 503)

switch timeidi

case 11 % (subfold == 503)

afa\_n = 0.15; %Ori: 0.15

N\_l = 1.3; %Ori: 5.0

gamma\_f = 0.04; %Ori: 0.04

gamma\_n = 0.00; %Ori: 0.0

beta\_f = 0.0; %Ori: 0.0

K\_s = 3.0e0; %uM %Ori: 3.0

afa\_f=0.18; %0.2; %0.15; %Ori:

Diff\_s = 0.01.\*1/3; %Ori: 0.003

gamma\_s = 0.02; %Ori:

case 21 % (subfold == 503)

afa\_n = 0.15; %Ori: 0.15

N\_l = 1.3; %Ori: 5.0

gamma\_f = 0.04; %Ori: 0.04

gamma\_n = 0.00; %Ori: 0.0

beta\_f = 0.0; %Ori: 0.0

K\_s = 3.0e0; %uM %Ori: 3.0

afa\_f=0.12; %0.15; %Ori:

Diff\_s = 0.008.\*1/3; %Ori: 0.003

gamma\_s = 0.02; %Ori:

case 31 % (subfold == 503)

afa\_n = 0.05; %Ori: 0.15

N\_l = 1.2; %Ori: 5.0

gamma\_f = 0.04; %Ori: 0.04

gamma\_n = 0.00; %Ori: 0.0

beta\_f = 0.0; %Ori: 0.0

K\_s = 3.0e0; %uM %Ori: 3.0

afa\_f=0.07; %0.15; %Ori:

Diff\_s = 0.005.\*1/3; %Ori: 0.003

gamma\_s = 0.02; %Ori:

otherwise

;

end

% afa\_n = 0.15; %Ori: 0.15

% N\_l = 1.3; %Ori: 5.0

%

% gamma\_f = 0.04; %Ori: 0.04

% gamma\_n = 0.00; %Ori: 0.0

% beta\_f = 0.0; %Ori: 0.0

% K\_s = 3.0e0; %uM %Ori: 3.0

% afa\_f=0.2; %0.15; %Ori:

% Diff\_s = 0.01; %Ori: 0.003

% gamma\_s = 0.02; %Ori:

elseif (subfold == 202)

%========== new parameters for 202 ====================

switch timeidi

case 11 % (subfold == 202)

afa\_n = 0.15; %Ori:

N\_l = 1.3; %Ori:

gamma\_f = 0.04; %Ori:

gamma\_n = 0.00; %Ori:

beta\_f = 0.0; %Ori:

K\_s = 3.0e0; %Ori:

afa\_f=1.15; %Ori:

Diff\_s = 0.25.\*1/3; %0.065; %Ori: 0.065

gamma\_s = 0.2; %Ori:

case 21 % (subfold == 202)

afa\_n = 0.15; %Ori:

N\_l = 1.3; %Ori:

gamma\_f = 0.04; %Ori:

gamma\_n = 0.00; %Ori:

beta\_f = 0.0; %Ori:

K\_s = 3.0e0; %Ori:

afa\_f=1.2; %Ori:

Diff\_s = 0.25.\*1/3; %0.065; %Ori: 0.065

gamma\_s = 0.2; %Ori:

case 31 % (subfold == 202)

afa\_n = 0.05; %Ori:

N\_l = 1.2; %Ori:

gamma\_f = 0.04; %Ori:

gamma\_n = 0.00; %Ori:

beta\_f = 0.0; %Ori:

K\_s = 3.0e0; %Ori:

afa\_f=0.40; %Ori:

Diff\_s = 0.16.\*1/3; %0.065; %Ori: 0.065

gamma\_s = 0.2; %Ori:

otherwise

;

end

end

% 60 mm plates instead of 90 mm plates

%Diff\_s = Diff\_s .\*1/3;

if subfold ==503

% %========== Original parameters ====================

% afa\_f=0.12;

% Diff\_s = 0.003; %0.4;

% gamma\_s = 0.02; %0.2;

% afa\_n = 0.075;

%========== New parameters ===========================

end

if subfold ==202

% %========== Original parameters ====================

% afa\_f=0.9;

% %Diff\_s = 0.065; %0.4;

% Diff\_s = 0.065; %0.4;

% gamma\_s = 0.2; %0.2;

% afa\_n = 0.11;

%========== New parameters ====================

end

if subfold ==503

switch timeidi

case 11

mean\_fluo0 = 95;

case 21

mean\_fluo0 = 117;

%mean\_fluo0 = 95;

case 31

mean\_fluo0 = 145;

%mean\_fluo0 = 95;

otherwise

;

end

elseif subfold ==202

switch timeidi

case 11

mean\_fluo0 = 31.94;

case 21

mean\_fluo0 = 30;

%mean\_fluo0 = 31.94;

case 31

%mean\_fluo0 = 35;

%mean\_fluo0 = 31.94;

mean\_fluo0 = 70;

otherwise

;

end

end

%===============================================

%Load initial conditions

%===============================================

U\_0 = 10.0e0; %mM

if subfold ==503

% %========== Original parameters ====================

% x0=0.3; %x0>=0

%========== New parameters ====================

%x0=1.2;

switch timeidi

case 11

x0=1.0; %1.2; %11

case 21

x0=0.9; %21

case 31

x0=0.83;

otherwise

;

end

end

if subfold ==202

% %========== Original parameters ====================

% x0=0.25;

%========== New parameters ====================

%x0=0.3;

switch timeidi

case 11

x0=0.3; %11

case 21

x0=1.0; %1.2; %21

case 31

x0=0.7;

otherwise

;

end

end

% 60mm plate instead of 90 mm plates

x0 = x0 .\*2/3;

U\_ini = U\_0./(x0.\*2) ;

%===============================================

%Boundary conditions

%===============================================

%===============================================

%Save parameter sets to a file

Para = [gamma\_f, gamma\_n, afa\_f, afa\_n, Diff\_s, gamma\_s, K\_s, N\_l, ...

U\_ini, x0, beta\_f];

%Para = [(1)gamma\_f, (2)gamma\_n, (3)afa\_f, (4)afa\_n, (5)Diff\_s, (6)gamma\_s,

%(7)K\_s, (8)N\_l, (9)U\_ini, (10)x0, (11)beta\_f];

fid = fopen('Para.txt', 'wt');

fprintf(fid, '%f\n', Para);

fclose(fid);

xl = -4.0 ;

xr = -xl ;

t0 = 0 ;

tf = 10 ;

%Nt\_step = 100 ;

Nt\_step = 1000 ;

%x = linspace(xl,xr,61);

x = linspace(xl,xr,61);

t = linspace(t0,tf,Nt\_step+1);

m = 0;

%sol = pdepe(m,@pdex1pde3,@pdex1ic3,@pdex1bc3,x,t);

sol = pdepe(m,@pdex1pde3,@pdex1ic3,@pdex1bc3,x,t);

S = sol(:,:,1);

F = sol(:,:,2);

N = sol(:,:,3);

%Total Fluo = Real Fluo + AutoFluorescence

%F = F + N.\*1.0;

%sol(:,:,2) = sol(:,:,2) + sol(:,:,3).\*1.0 ;

F\_tot = F + sol(:,:,3).\*1.0 ;

%Plot the simulated results

figure(100)

subplot(2,2,1)

h1=surf(x,t,S);

title(['Numerical solution computed: S (AHL)']);

xlabel('Distance x');

ylabel('Time t');

set(h1,'linestyle', 'none');

%colorbar

view(2) % view in 2D

subplot(2,2,2)

h1=surf(x,t,F\_tot);

title(['Numerical solution computed: F (Fluores)']);

xlabel('Distance x');

ylabel('Time t');

set(h1,'linestyle', 'none');

view(2)

subplot(2,2,3)

h1=surf(x,t,N);

title(['Numerical solution computed: N (Cell Den)']);

xlabel('Distance x');

ylabel('Time t');

set(h1,'linestyle', 'none');

view(2)

%Plot the simulated time evolution of fluorescence intensity

figure(200)

%figure,

%subplot(2,2,4)

%figure,

Nk = 5 ;

Nsize = floor(Nt\_step/Nk) ;

%F.P.

color=['r', 'm', 'g', 'b', 'k', 'ko', 'kx'];

%Time points where images were taken

%X\_val=[0; 29; 55; 92]+1; % Time points for the 2009 experiments

%! it seems that for strain 202, X\_val=[0; 15; 50; 80]+1 is better than X\_val=[0; 25; 50; 80]+1;

% while for Strain 503, X\_val=[0; 25; 50; 80]+1 is good.

X\_val=[0; 25; 50; 80]+1;

if subfold == 503

% X\_val=[0; 25; 50; 80]+1;

X\_val=[0; 250; 500; 800]+1;

elseif subfold == 202

% X\_val=[0; 15; 50; 80]+1;

X\_val=[0; 150; 500; 800]+1; % Seems like there’s a delay

end;

%X\_val=[0; 15; 50; 80]+1;

%X\_val=[0; 25; 50; 80]+1; % Time points for the 2015 experiments

% one time step = 0.1 hr.

for k=1:4

plot(x,F\_tot(X\_val(k),:),[color(k) '-']);

hold on;

end

title(['Fluoresence in different time: ' ...

'D\_s=' num2str(Diff\_s) ', \gamma\_s=' num2str(gamma\_s) ',K\_s=' num2str(K\_s) ] );

xlabel('Distance x')

ylabel('Fluoscence (a.u.)')

axis([-4 4 -0.2 max(max(F\_tot(:,:))) ]);

box on;

%Plot the comparison between experiments and simulations

figure('Position', [200, 300, 1500, 600]);

%experimental data

subplot(1,2,1)

% timeidi = 11;

% timeidf = 14;

for timeid = timeidi:1:timeidf

%Read & plot the experimental data.

formatSpec = '%f %f\n';

sizeA = [2 Inf];

fp=fopen(['.\ActualRun20151101\' num2str(subfold), '-', num2str(timeid), '.txt'],'r');

A = fscanf(fp,formatSpec,sizeA);

fclose(fp);

A = A';

mean\_color = ['r', 'm', 'g', 'b'];

color\_ind = mean\_color(mod(timeid,10));

title(['Original Experimental Fluorescence over Time: ', '[Strain-', num2str(subfold), ']']);

xlabel('Distance X (cm)');

ylabel('Fluoscence (a.u.)');

plot(A(:,1),A(:,2),color\_ind);

A=[];

grid on; hold on;

% if (timeid == timeidi)

% mean\_fluo0 = mean(A(:,2));

% end

end

axis([-4 4 0 300 ]);

box on;

%simulated results

subplot(1,2,2)

for k=1:4

plot(x,F\_tot(X\_val(k),:),[color(k) '-']);

hold on;

end

title(['Fluoresence in different time: ' ...

'D\_s=' num2str(Diff\_s) ', \gamma\_s=' num2str(gamma\_s) ',K\_s=' num2str(K\_s) ] );

xlabel('Distance X (cm)')

ylabel('Fluoscence (a.u.)')

axis([-4 4 -0.2 max(max(F\_tot(:,:))) ]);

box on; grid on;

% fig = gcf;

%FigHandle = figure('Position', [200, 300, 1500, 600]);

%Plot the comparison between experiments and simulations

%figure('Position', [200, 300, 1500, 600]);

figure('Position', [200, 300, 750, 300]);

%experimental data

subplot(1,2,1)

for timeid = timeidi:1:timeidf

%Read & plot the experimental data.

formatSpec = '%f %f\n';

sizeA = [2 Inf];

fp=fopen(['.\ActualRun20151101\' num2str(subfold), '-', num2str(timeid), '.txt'],'r');

A = fscanf(fp,formatSpec,sizeA);

fclose(fp);

A = A';

mean\_color = ['r', 'm', 'g', 'b'];

color\_ind = mean\_color(mod(timeid,10));

plot(A(:,1).\*2/3,A(:,2)./mean\_fluo0,color\_ind, 'linewidth', 1.0);

if subfold == 503

maxY = 2.6;

elseif subfold == 202

maxY = 8.0;

end

%axis([-4 4 0 maxY]);

axis([-3 3 0 maxY]);

%axis([-4 4 0 max(max(F\_tot(:,:)))]);

%title(['Experimental Fluorescence over Time: ', '[Strain-', num2str(subfold), ']']);

%title(['Experimental Fluorescence over Time: ', '[Strain-', ...

% num2str(subfold), '; Time=', num2str(timeidi),'-', num2str(timeidf) ']']);

title(['Experiment']);

xlabel('Distance X (cm)')

ylabel('Normalized Fluoscence (a.u.)')

%grid on;

hold on;

end

%simulated results

subplot(1,2,2)

for k=1:4

plot(x,F\_tot(X\_val(k),:),[color(k) '-'],'linewidth', 1.5);

hold on;

end

%title(['Simulated Fluoresence over Time ', '[Strain-', num2str(subfold), '], ' ...

% 'D\_s=' num2str(Diff\_s) ', \gamma\_s=' num2str(gamma\_s) ',K\_s=' num2str(K\_s) ] );

title(['Simulation']);

xlabel('Distance x')

ylabel('Fluoscence (a.u.)')

axis([-3 3 0 maxY]);

%axis([-4 4 0 maxY]);

%axis([-4 4 0 max(max(F\_tot(:,:))) ]);

box on;

%grid on;

%Plot the comparison between experiments and simulations

figure('Position', [600, 300, 700, 600]);

for timeid = timeidi:1:timeidf

%Read & plot the experimental data.

formatSpec = '%f %f\n';

sizeA = [2 Inf];

fp=fopen(['.\ActualRun20151101\' num2str(subfold), '-', num2str(timeid), '.txt'],'r');

A = fscanf(fp,formatSpec,sizeA);

fclose(fp);

A = A';

mean\_color = ['r', 'm', 'g', 'b'];

color\_ind = mean\_color(mod(timeid,10));

%experimental data

% plot(A(:,1),A(:,2)./mean\_fluo0,color\_ind);

% 60 mm plates instead of 90 mm.

plot(A(:,1).\*2/3,A(:,2)./mean\_fluo0,color\_ind);

if subfold == 503

maxY = 2.6;

elseif subfold == 202

maxY = 8.0;

end

axis([-4 4 0 maxY]);

%axis([-4 4 0 max(max(F\_tot(:,:)))]);

title(['Experimental Fluorescence over Time: ', '[Strain-', ...

num2str(subfold), '; Time=', num2str(timeidi),'-', num2str(timeidf) ']']);

xlabel('Distance X (cm)')

ylabel('Normalized Fluoscence (a.u.)')

grid on; hold on;

end

%simulated data

for k=1:4

hold on; plot(x,F\_tot(X\_val(k),:),[color(k) '-']);

end