Ransford Antwi

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EGR102

Final Project Part 3: Simulate Actual Data from Bioreactor vs Predicted Data and

Calculate MSE

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Due: Wednesday at Midnight April 17th, 2024

The assignment is to simulate a BIOREACTOR WITH SUBSTRATE INHIBITION.

You will be building off this system to

1. Simulate the continuous bioreactor for a time frame with fixed inputs.
2. Simulate the continuous bioreactor with a step response in flow rate.
3. Simulate actual data vs predicted data and calculate mean square error.
4. Fit baseline maximum growth rate, µmax (mu\_max), given set of data.
5. Fit growth kinetics for max growth rate µmax, the Monod Constant, K, and inhibition factor Ki.

EC) Optimize Fin for best production.

Modeling Equations:

Note: growth rate µ(mu) should be in the ODE function file.

*Please note that all user assigned values highlighted yellow are changes from part 2 that you should make in your part 3 ic file!*

% Simulation Parameters

*Obtain from data file: t\_end, delt*

% Initial Conditions:

X(1)= 161.916;% g cells/ L

S(1)= 7.125;% g substrate/ L

P(1)= 80.96;% g protein /L

*Obtain from data file: X\_act*

%Nominal Parameter Values (To Be Fitted):

mu\_max = 0.5;% maximum growth rate h-1

K= 20;% Monod growth constant g substrate/L

Ki= 50;% Substrate inhibition growth constant g substrate/L

% Input

*Obtain from data file: Fin\_act*

% Parameters:

V=1000;% bioreactor volume L

YSX = 1.5;% yield g substrate/ g cells

YPX = 0.5;% yield g protein/ g cells

Xin = 0;% feed biomass concentration g cells/L

Sin = 250;% feed substrate concentration g substrate/L

Pin = 0;% feed protein concentration g protein/L

1. Build off the part 2 ic file done earlier. Rename so part 3.
   1. Load the mat file. load final\_proj\_data
   2. Use the sample time and total time from the mat file. So delete delt and t\_end.
   3. Set Fin=Fin\_act assume inputs used to generate the actual data are correct and accurate.
   4. Prior to for loop initialize sum of square error SSE=(X\_act(1)-X(1))^2 (sum of square error)
   5. Just prior to ending the for loop calculate the sum of square error

SSE=SSE+ (X\_act(i)-X(i))^2

* 1. After all data is run and for loop is completed, calculate the mean square error. MSE= SSE/N

1. Generate one figure with 3 subplots:
   1. Title should be: Final Project Practice Part 3 MSE= “MSE” with k0= “k0” and Ea=”Ea” NOTE:”” are embedded parameters
   2. t vs Ca as green circles

t\_act vs Ca\_act as black diamonds

legend “Predicted” “Actual”

with yaxis “Ca (moles A/L)”

* 1. t vs T with yaxis “T (Celsius)”
  2. t vs D with yaxis “D 1/hr” and xaxis “Time (hrs)”

Paste here the following:

1. final\_project\_pract\_part3\_ic.m file
2. figure generated

Save all files since will be building on these for subsequent parts!

1. Generate one figure with 4 subplots:
   1. Title should be: Final Project Part 3 MSE= “MSE” with mu max= “mu\_max”, K=”K” , and Ki=”Ki” NOTE:”” are embedded parameters
   2. t vs X as red crosses

t\_act vs X\_act as black diamonds

legend “Predicted” “Actual”

with yaxis “X (g cells/L)”

* 1. t vs S with yaxis “S (g substrate/L)”
  2. t vs P with yaxis “P (g protein/L)”
  3. t vs Fin with yaxis “Fin (L/hr)” and xaxis “Time (hrs)”

Paste here the following:

1. final\_project\_part3\_ic.m file
2. final\_project\_ode.m file
3. figure generated

Save all files since will be building on these for subsequent parts!

*If done correctly should get figure similar to this:*

A screenshot of a graph

Description automatically generated

1. .
2. final\_project\_pract\_part3\_ic.m file

% final\_proj\_pract3\_ic.m

% Ransford Antwi

% 16 April 2024

%

%

% States in Original Van de vusse: Ca Cb

% States in Final Proj Practice Ca and T

% Parameters in Original van de vusse: k1,k2,k3

% Parameters in Final Proj Practice:

% Caf, Tf,k0,Ea,R,minus\_delH,rho, cp, U, A, V

%

% Blank slate

clear

clc

% User Assigned

%loading the atual data

load final\_proj\_pract\_data

% Initial Conditions ba

Ca(1)=1.0843; % concentration of A in reactor moles A/L

T(1)=418.0618; % reactor temperature in Celsius

% Simulation Param

%BA getting samlple time and total

% t\_end=20; % simulation time hours

% t\_step=2;% BA time step response occurs in hrs

% delt=0.04;% BA sample time in hrs

% D\_init=0.2;

% D\_final=0.22;

% Parameters: ba

Caf=20;% feed concentration of A in moles A/L feed

Tf=30;% temperature of feed into reactor in degrees Celsius

R=8.314;% gas constant in J/K-mol

minus\_delH=9E6;% heat of reaction J mol^-1

rho=1000;% density in kg/m^3

cp=420;% Heat capacity in J/kg/C

U=1.8E3;% heat transfer coefficient in J/m^2/K/hr

A=2; % jacket area in m^2

V=1;% reactor volume in m^3

% Will be Fitted Parameters ba

k0=7;% base kinetic rate constant in 1/hr

Ea=4000;% activation energy in J

% Inputs

% BA added

D=D\_act;

Tj=15;% jacket temperature in Celsius

% Main Program

x0=[Ca(1);T(1)];% ba initialization vector

% Pack these into Param vector ba

Param(1)=Caf;% feed concentration of A in moles A/L feed

Param(2)=Tf;% temperature of feed into reactor in degrees Celsius

Param(3)=R;% gas constant in J/K-mol

Param(4)=minus\_delH;% heat of reaction J mol^-1

Param(5)=rho;% density in kg/m^3

Param(6)=cp;% Heat capacity in J/kg/C

Param(7)=U;% heat transfer coefficient in J/m^2/K/hr

Param(8)=A; % jacket area in m^2

Param(9)=V;% reactor volume in m^3

% BA Now calculate samples in for loop

N=ceil(t\_end/delt); % BA rounds up any remainder to next highest integer

% BA save initial time point and input

t(1)=0;

%intial sum of square

SSE=(Ca\_act(1)-Ca(1))^2;

% D(1)=D\_init;

for i=2:N

t(i)=t(i-1)+delt;% BA time vector

% xdot=final\_proj\_pract1\_ode(t,x,opts,Param,k0,Ea,D,Tj)

[~,Xout]=ode45('final\_proj\_pract1\_ode',[t(i-1) t(i)],x0,[],Param,k0,Ea,D(i-1),Tj);%ode45 call params,inputs passed at end

% BA save only last data point for our ith sample!

Ca(i)=Xout(end,1);% ba Ca is the first state in x0 and xdot its derivative is 1st

T(i)=Xout(end,2);%ba T is 2nd

% BA reinitialize your states.

x0=[Ca(i);T(i)];% ba initialization vector

%BA cal sum of sq error

SSE=SSE+(Ca\_act(i)-Ca(i))^2;

end

MSE=SSE/N; %Mean square error divide total by numebr sample

figure(1) % Now include the input too!

subplot(3,1,1);plot(t,Ca,'go',t\_act,Ca\_act,'kd')

title(['Final Project Practice Part 3 with MSE=',num2str(MSE),'with K0=',num2str(k0),' and Ea=',num2str(Ea)])

legend('Predicted','Actual')

ylabel('Ca moles A/L')% ba

subplot(3,1,2);plot(t,T)% ba

ylabel('T (Celsius)')

subplot(3,1,3);plot(t,D)% ba

ylabel('D 1/hr')

xlabel('Time(hrs)')

2). Figure generated



1. .

3). final\_project\_pract\_part3\_ic.m file

%Bioreactor\_actual/predic\_MSE\_ic%

%Ransford Antwi%

%March 5, 2024%

%Final\_Project\_Part\_3\_main

%blank slate%

clear

clc

% user assigned%

%loading data file

load final\_proj\_3\_data\_file.mat

% Simulation Parameters

% will obtain from data file instead

% Initial Conditions:

X(1)= 161.916;% g cells/ L

S(1)= 7.125;% g substrate/ L

P(1)= 80.96;% g protein /L

%Nominal Parameter Values (To Be Fitted):

mu\_max = 0.5;% maximum growth rate h-1

K= 20;% Monod growth constant g substrate/L

Ki= 50;% Substrate inhibition growth constant g substrate/L

%input added

Fin=Fin\_act;

%Parameters

V=1000;% bioreactor volume L

Ysx = 1.5;% yield g substrate/ g cells

Ypx = 0.5;% yield g protein/ g cells

Xin = 0;% feed biomass concentration g cells/L

Sin = 250;% feed substrate concentration g substrate/L

Pin = 0;% feed protein concentration g protein/L

%main program

%[xdot]=lorenz\_ode\_2(t,x,opts,sigma,r,b)

%intialization

x0=[X(1);S(1);P(1);];

%unpacking to various parameters

param(1)=V;

param(2)=Ysx;

param(3)=Ypx;

param(4)=Xin;

param(5)=Sin;

param(6)=Pin;

param(7)=K;

param(8)=Ki;

%initial time

t(1)=0;

%number of samples in for loop

N=ceil(t\_end/delt);

%intial sum of square

SSE=(X\_act(1)-X(1))^2;

for i=2:N

t(i)=t(i-1)+delt;

%[xdot]=vdv\_fxn(t,x,opts,param,u)

[~,Xout]=ode45('Bioreactor\_fxn',[t(i-1) ,t(i)],x0,[],param,Fin(i-1),mu\_max);

%unpack Xout to common notation for states

X(i)=Xout(end,1);

S(i)=Xout(end,2);

P(i)=Xout(end,3);

% ba initialization vector

x0=[X(i);S(i);P(i)];

%BA call sum of sq error

SSE=SSE+(X\_act(i)-X(i))^2;

end

MSE=SSE/N; %Mean square error divide total by numebr sample

%Graphing

%ploting subplot

figure(1);

subplot(4,1,1);plot(t,X,'rx',t,X\_act,'kd')

ylabel('X(g cells/L')

legend('Predicted','Actual')

title(['Final Project Part 3 MSE=',num2str(MSE),' with mumax=',num2str(mu\_max),'K=',num2str(K),'and Ki=',num2str(Ki)])

subplot(4,1,2);plot(t,S)

ylabel('S(g substrate/L')

subplot(4,1,3);plot(t,P)

ylabel('P(g Protein/L')

subplot(4,1,4);plot(t,Fin)

ylabel('Fin(g L/hr)')

xlabel('Time(hrs)')

4). final\_project\_ode.m file

%Bioreactor\_fxn\_ode

%Ransford Antwi

%user assigned

% Simulation Parameters

% t\_end=100; % total simulation hrs

%

% % Initial Conditions:

% X(1)= 0.1;% g cells/ L

% S(1)= 20;% g substrate/ L

% P(1)= 0;% g protein /L

%

% %Nominal Parameter Values (To Be Fitted):

% mu\_max = 0.5;% maximum growth rate h-1

% K= 20;% Monod growth constant g substrate/L

% Ki= 50;% Substrate inhibition growth constant g substrate/L

% Input

%Fin=100;% feed flow rate L/hr

% Parameters

% V=1000;% bioreactor volume L

% YSX = 1.5;% yield g substrate/ g cells

% YPX = 0.5;% yield g protein/ g cells

% Xin = 0;% feed biomass concentration g cells/L

% Sin = 80;% feed substrate concentration g substrate/L

% Pin = 0;% feed protein concentration g protein/L

%main program

function [xdot]=bioreactor\_ode(t,x,opts,param,Fin,mu\_max)

X=x(1); %position must match

S=x(2);

P=x(3);

%packing elements to param

V=param(1);

Ysx=param(2);

Ypx=param(3);

Xin=param(4);

Sin=param(5);

Pin=param(6);

K=param(7);

Ki=param(8);

%ODE

mu=mu\_max\*S/(K+S+(S^2/Ki));

dXdt=(Fin\*(Xin-X))/V+mu\*X;

dSdt=(Fin\*(Sin-S))/V-Ysx\*mu\*X;

dPdt=(Fin\*(Pin-P))/V+Ypx\*mu\*X;

xdot=[dXdt;dSdt;dPdt];

Figure Generated

