EGR 103L – Fall 2017

Laboratory 8 - Intermediate Curve Fitting

Ian Hanus (ih52)
Lab Section 1B, Tuesday 8:30-11:2-
November 12th, 2017

I have adhered to the Duke Community Standard in completing this assignment. I understand that a violation of the Standard can result in failure of this assignment, failure of this course, and/or suspension from Duke University.

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1 Palm 6.9

$S_T = 2.0361e+03$

Order	Coefficients P of $T = f(A) = \sum_{k=1}^{\text{Order}+1} P(k)A^{(\text{Order}+1-k)}$	S_r	r^2
1	[-6.9697e-01 1.0844e+02]	1.9960e+03	1.9683e-02
2	[-1.9053e+00 -1.7845e+01 1.3130e+02]	7.9289e+01	9.6106e-01
3	[1.0684e-02 1.7611e+00 -1.7352e+01 1.3103e+02]	7.8937e+01	9.6123e-01
4	[-2.4913e-02 4.5911e-01 -7.5510e-01 -1.2868e+01 1.2995e+02]	6.8713e+01	9.6625e-01

The minimum drying times and additive amounts for each fit are:

Order	Min. Drying Time (min)	A for Min. Drying Time (oz)
1	8.9999e+00	1.0216e+02
2	8.9518e+01	4.6829e+00
3	8.9486e+01	4.7236e+00
4	8.8304e+01	4.6765e+00

2 Palm 6.16

$$y(x) = (5.7518e+00) + (9.9123e+00)\ln(x)$$

The statistical information is:

$S_t = 4.8359e+00$ $\qquad$ $S_r = 3.0297e+03$ $\qquad$ $r^2 = -6.2550e+02$

The estimates asked for using this model are:

$y(2.5) \approx 2.4292e+01$ $\qquad$ $y(11) \approx 7.3182e+01$

3 Chapra 15.7

Based on the least-squares fit of the given models,

$$OC(c,T) = (1.4027e+01) - (1.4027e-01) - (3.3642e-01)T - (1.0493e-01)T^2 + (1.4027e+01)T^3$$

For this model with these data points,

$S_t = 1.0400e+02$ $\qquad$ $S_r = 1.2784e+00$ $\qquad$ $r^2 = 9.8771e-01$

Because the r^2 value is so close to 1, above 0.95, this is model provides a good mathematical fit for the data. The estimate of $OC(15,12)$ is 9.1678e+00 mg/L, which has a relative error of (8.5605e-01)% from the known value.

4 Chapra 15.10

Based on the least squares fit of the given model,

$$p(t) = (4.1375e+00)e^{-1.5t} + (2.8959e+00)e^{-0.3t} + (1.5349e+00)e^{-0.05t}$$

The statistical and specific information required by the problem is:

A	B	C	S_T	S_r	r^2
$4.1375e+00$	$2.8959e+00$	$1.5349e+00$	$2.0409e+01$	$8.0348e-02$	$9.9606e-01$

Because the r^2 value is so close to one, above 0.95, this model is a good mathematical fit for the data.

5 Chapra 15.10 Alternate

Based on the least squares fit of the given model,

$$p(t) = (5.6328e + 00)e^{-1.5t} - (4.4272e + 00)e^{-0.3t} + (7.8906e + 00)e^{-0.2t}$$

The statistical and specific information required by the problem is:

A	B	C	S_t	S_r	r^2
5.6328e+00	-4.4272e+00	7.8906e+00	2.0409e+01	7.9611e-02	9.9610e-01

Because the r^2 value is so close to one, above 0.95, this model is a good mathematical fit for the data.

6 Chapra 15.12

$$y(x) = (3.745e - 01) + (9.8644e - 01)x + \frac{8.4564e - 01}{x}$$

The statistical information is:

$$S_t = 6.9480e + 00 \qquad S_r = 2.7651e - 03 \qquad r^2 = 9.9960e - 01$$

The estimates asked for using this model are:

$$y(1.5) \approx 2.4179e + 00 \qquad y(4.5) \approx 5.0014e + 00$$

7 Chapra 15.11

The model equation is:

$$P = P_m \frac{I}{I_{sat}} e^{-\frac{I}{I_{sat}} - 1} = (2.3871e + 02) \frac{I}{2.2182e + 02} e^{-\frac{I}{2.2182e+02} - 1}$$

with P_m measured in (mg m^{-3} d^{-1}) and I_{sat} measured in (μE m^{-2}s^{-1}).

$$S_r = 1.1159e + 03$$
$$S_t = 2.8370e + 04$$
$$r^2 = 9.6067e - 01$$

Because the r^2 value is so close to 1, above 0.95, this model is a good mathematical fit for the data given. The initial guesses came from the maximum photosynthesis rate given in the tale and the I value that was near it.

8 Chapra 15.14

The S_t for the data set is 1.0847e-09. With a model of:

$$v_0 = \frac{(2.4310e - 05)[S]^3}{(3.9977e - 01) + [S]^3}$$

$$S_r = 2.1212e - 18$$
$$S_t = 1.0847e - 09$$
$$r^2 = 1.0000e + 00$$

Because r^2 is equal to one, this model is a perfect fit for the data. The initial guesses for k_m and S came from the limit ofv_0 as S went to infinity and the S^3 value at about half of the v_0 maximu.

A Codes and Output

A.1 Paint.m

```
 % I have adhered to all the tenets of the
 % Duke Community Standard in creating this code.
 % Signed: [ih52]

%% Setup function
function [P, Sr, r2, Amin, Tmin] = Paint(A, T, Order)

%% Setup equations
P = polyfit(A, T, Order)
That = polyval(P, A);
St = sum((T - mean(T)).^2)
Sr = sum((T-That).^2)
r2 = (St - Sr)/St

%% Find minimum drying time and amount of additive
[Amin, Tmin] = fminbnd(@(Adummy) polyval(P,Adummy) ,0,9)


```

A.2 Palm6p9.m

```
 % I have adhered to all the tenets of the
 % Duke Community Standard in creating this code.
 % Signed: [ih52]

A = 0:1:9;
T = [130 115 110 90 89 89 95 100 110 125];

[P1,Sr,r2,Amin1,Tmin1] = Paint(A,T,1)
[P2,Sr,r2,Amin2,Tmin2] = Paint(A,T,2)
[P3,Sr,r2,Amin3,Tmin3] = Paint(A,T,3)
[P4,Sr,r2,Amin4,Tmin4] = Paint(A,T,4)
%% Plot the graphs
A1 = linspace(0,9,100);
figure(1); clf
plot(A1,polyval(P1,A1),'k-')
hold on
plot(A1, polyval(P2,A1),'k.-')
plot(A1, polyval(P3,A1),'k--')
plot(A1, polyval(P1,A1),'k:')
plot(A,T,'ms')
hold off
gzoom
title ('Drying Time of Paint with Varying Amounts of Additive (ih52)')
xlabel('Additive (oz)')
ylabel('Time (min)')
legend('1st Order', '2nd Order', '3rd Order', '4th Order')
print -depsc Palm6p9plot
```

A.3 Palm6p16.m

```
 % I have adhered to all the tenets of the
 % Duke Community Standard in creating this code.
 % Signed: [ih52]

%% Configure workspace
clear; format short e

%% Establish values
x = 1:1:10;
y = [10 14 16 18 19 20 21 22 23 23];

%% Find curve fit and other values
x = log(x);
Pfit = polyfit(x,y,1)
Pval = polyval(Pfit, x);
St = sum((x-mean(x)).^2)
Sr = sum((x-Pval).^2)
r2 = (St-Sr)/St

%% Calculate estimates
Val25 = polyval(Pfit, 2.5)
Val11 = polyval(Pfit, 11)
```

A.4 Chapra15p7.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [General Linear Regression]
% Written by: [Dr. Gustafson]

% I understand and have adhered to all the tenets of the
% Duke Community Standard in creating this code.  I understand
% that a violation of any part of the Standard on any part of
% this assignment can result in failure of this assignment,
% failure of this course, and/or suspension from Duke University.
% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Load data and split into matrices and vectors
load DocTable.mat
cm = c; cv = c(:);
Tm = T; Tv = T(:);
OCm = OC; OCv = OC(:);

%% Determine coefficients using multiple linear regression
yeqn = @(coefs, cval, tval) coefs(1)*tval.^3 + coefs(2)*tval.^2 + coefs(3)*tval.^1 + coefs(4)*cval.^1 +
A =                                    [Tv.^3              Tv.^2              Tv.^1              cv.^1
MyCoefs = A\OCv

%% Create meshgrid and surface plot
figure(1);clf
MinT = min(T(:)); MaxT = max(T(:)); Tmesh = linspace(MinT,MaxT,19);
Minc = min(c(:)); Maxc = max(c(:)); Cmesh = linspace(Minc,Maxc,17);
[cmodel, Tmodel] = meshgrid(Tmesh,Cmesh);
OCmodel = yeqn(MyCoefs,cmodel,Tmodel);
surfc(cmodel, Tmodel, OCmodel)
view(145,15)
xlabel('Chloride Concentration (mg/L)')
ylabel('Temperature (C)')
zlabel('Oxygen Concentration (mg/L)')
title('Concentration of Oxygen at Given Temperatures and Chloride Concentrations')
colormap autumn
print -depsc Chapra15p7plot
%% Determine St, Sr, and r2 values of model
OChat = yeqn(MyCoefs, cv, Tv);
St = sum((OCv - mean(OCv)).^2)
Sr = sum((OCv - OChat).^2)
r2 = (St - Sr)/St

%% Estimate for c = 15 and T = 12, with percent error
OCestimate = yeqn(MyCoefs,15,12)
PercentError = abs(OCestimate - 9.09)/9.09*100
```

A.5 Chapra15p10.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [General Linear Regression]
% Written by: [Dr. Gustafson]

% I understand and have adhered to all the tenets of the
% Duke Community Standard in creating this code.  I understand
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% this assignment can result in failure of this assignment,
% failure of this course, and/or suspension from Duke University.
% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Determine coefficients using general linear regression
t = [0.5 1 2 3 4 5 6 7 9];
tv = t(:);
Pt = [6 4.4 3.2 2.7 2 1.9 1.7 1.4 1.1];
Ptv = Pt(:);
yeqn = @(coefs, dummyt) coefs(1)*exp(-1.5*dummyt) + coefs(2)*exp(-0.3*dummyt) + coefs(3)*exp(-0.05*dummy
A = [exp(-1.5*tv) exp(-0.3*tv)  exp(-0.05*tv)];
MyCoefs = A\Ptv

%% Generate a model and plot
tmodel = linspace(min(t),max(t),100);
Ptmodel = yeqn(MyCoefs, tmodel);
plot(tmodel,Ptmodel,'k-',t,Pt,'b+')
xlabel('Time (s)'); ylabel('Organism Decay (organisms/cm^3'); title('Disease Carrying Organism Decay')
print -depsc Chapra15p10plot1

%% Plot concentrations of organisms
figure(2); clf
ConcA = MyCoefs(1)*exp(-1.5*tmodel);
ConcB = MyCoefs(2)*exp(-0.3*tmodel);
ConcC = MyCoefs(3)*exp(-0.05*tmodel);
plot(tmodel,ConcA,'k-',tmodel,ConcB,'k-.',tmodel,ConcC,'k--')
legend('Species A','Species B','Species C')
print -depsc Chapra15p10plot2

%% Determine St, Sr, and r2 values
Pthat = yeqn(MyCoefs,t)
St = sum((Pt - mean(Pt)).^2)
Sr = sum((Pt - Pthat).^2)
r2 = (St - Sr)/St
```

A.6 Chapra15p10alt.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [General Linear Regression]
% Written by: [Dr. Gustafson]

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% failure of this course, and/or suspension from Duke University.
% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Determine coefficients using general linear regression
t = [0.5 1 2 3 4 5 6 7 9];
tv = t(:);
Pt = [6 4.4 3.2 2.7 2 1.9 1.7 1.4 1.1];
Ptv = Pt(:);
yeqn = @(coefs, dummyt) coefs(1)*exp(-1.5*dummyt) + coefs(2)*exp(-0.3*dummyt) + coefs(3)*exp(-0.2*dummyt
A = [exp(-1.5*tv) exp(-0.3*tv)  exp(-0.2*tv)];
MyCoefs = A\Ptv

%% Generate a model and plot
figure(1);clf
tmodel = linspace(min(t),max(t),100);
Ptmodel = yeqn(MyCoefs, tmodel);
plot(tmodel,Ptmodel,'k-',t,Pt,'b+')
xlabel('Time (s)'); ylabel('Organism Decay (organisms/cm^3'); title('Disease Carrying Organism Decay')
print -depsc Chapra15p10altplot1

%% Plot concentrations of organisms
figure(2); clf
ConcA = MyCoefs(1)*exp(-1.5*tmodel);
ConcB = MyCoefs(2)*exp(-0.3*tmodel);
ConcC = MyCoefs(3)*exp(-0.05*tmodel);
plot(tmodel,ConcA,'k-',tmodel,ConcB,'k-.',tmodel,ConcC,'k--')
legend('Species A','Species B','Species C')
print -depsc Chapra15p10altplot2

%% Determine St, Sr, and r2 values
Pthat = yeqn(MyCoefs,t)
St = sum((Pt - mean(Pt)).^2)
Sr = sum((Pt - Pthat).^2)
r2 = (St - Sr)/St
```

A.7 Chapra15p12.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [General Linear Regression]
% Written by: [Dr. Gustafson]

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% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Enter given data and put into columns
x = 1:5;
y = [2.2 2.8 3.6 4.5 5.5];
xv = x(:);
yv = y(:);

%% Determine coefficients
yeqn = @(coefs,x) coefs(1)*x.^0+coefs(2)*x.^1+coefs(3)*x.^(-1);
A =                          [xv.^0         xv.^1        xv.^(-1)];
MyCoefs = A\yv

%% Build model
xmodel = linspace(min(x),max(x),100);
ymodel = yeqn(MyCoefs,xmodel);

%% Find St, Sr, and r2
yhat = yeqn(MyCoefs,xv);
St = sum((yv - mean(y)).^2)
Sr = sum((yv - yhat).^2)
r2 = (St-Sr)/St

%% Estimate values of x = 1.5 and x = 4.5
X15est = yeqn(MyCoefs,1.5)
X45est = yeqn(MyCoefs,4.5)
```

A.8 Chapra15p11.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [Nonlinear Regression]
% Written by: [Dr. Gustafson]

% I understand and have adhered to all the tenets of the
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% that a violation of any part of the Standard on any part of
% this assignment can result in failure of this assignment,
% failure of this course, and/or suspension from Duke University.
% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Express given data
I = [50 80 130 200 250 350 450 550 700];
P = [99 177 202 248 229 219 173 142 72];
Iv = I(:);
Pv = P(:);

%% Determine function coefficients
Peqn = @(coefs,I) coefs(1).*I./coefs(2).*exp(-I./coefs(2)+1)
fSSR = @(coefs,I,P) sum((P-Peqn(coefs,I)).^2);
[MyCoefs,Sr] = fminsearch(@(MyCoefsdummy) fSSR(MyCoefsdummy,Iv,Pv),[250 250])

%% Plot
figure(1); clf
Imodel = linspace(min(I),max(I),100);
Pmodel = Peqn(MyCoefs,Imodel);
plot(Imodel,Pmodel,'k',I,P,'rd')
xlabel('Solar Radiation (\muEm^(-2)^s(-1))')
ylabel('Photosynthesis Rate (mg m^(-3)d^(-1)')
title('Photosyntehsis Rate as a function of Solar Radiation (ih52)')
print -depsc Chapra15p11plot

%% Statistical measures
St = sum((P - mean(P)).^2)
r2 = (St-Sr)/St
```

A.9 Chapra15p14b.m

```
% [Chapra15p14b.m]
% [Ian Hanus]
% [11/12/17]
% Based on: [Nonlinear Regression]
% Written by: [Dr. Gustafson]

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% that a violation of any part of the Standard on any part of
% this assignment can result in failure of this assignment,
% failure of this course, and/or suspension from Duke University.
% Signed: [ih52]

%% Initialize workspace
clear; format short e

%% Load data
S = [0.01 0.05 0.1 0.5 1 5 10 50 100];
v0 = [6.078e-11 7.595e-9 6.063e-8 5.788e-6 1.737e-5 2.423e-5 2.430e-5 2.431e-5 2.431e-5];
Sv = S';
v0v = v0';

%% Determine coefficients
v0eqn = @(coefs,Sv) coefs(1).*Sv.^3./(coefs(2)+Sv.^3);
fSSR = @(coefs,Sv,v0v) sum((v0v - v0eqn(coefs,Sv)).^2)
[MyCoefs, Sr] = fminsearch(@(MyDummyCoefs) fSSR(MyDummyCoefs,Sv,v0v),[2.431e-5 5])
St = sum((v0v-mean(v0v)).^2)
r2 = (St-Sr)/St

%% Plots
figure(1); clf
Smodel = linspace(min(S), max(S), 100);
v0model = v0eqn(MyCoefs,Smodel);
plot(Smodel,v0model,'k-',S,v0,'ro')
xlabel('Substrate Concentration (M)')
ylabel('Initial Rate of Reaction (M/s)')
title('Rate of Enzymatic Reactions (ih52)')
print -depsc Chapra15p14bplot

figure(2); clf
loglog(Smodel,v0model,'k-',S,v0,'ro')
xlabel('log(Substrate Concentration (M))')
ylabel('log(Initial Rate of Reaction (M/s))')
title('Log of Rate of Enzymatic Reactions (ih52)')
print -depsc Chapra15p14blogplot
```

B Figures

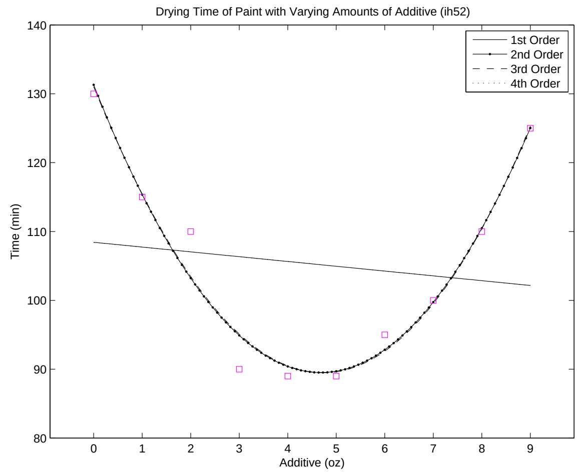

Figure 1: Palm 6.9

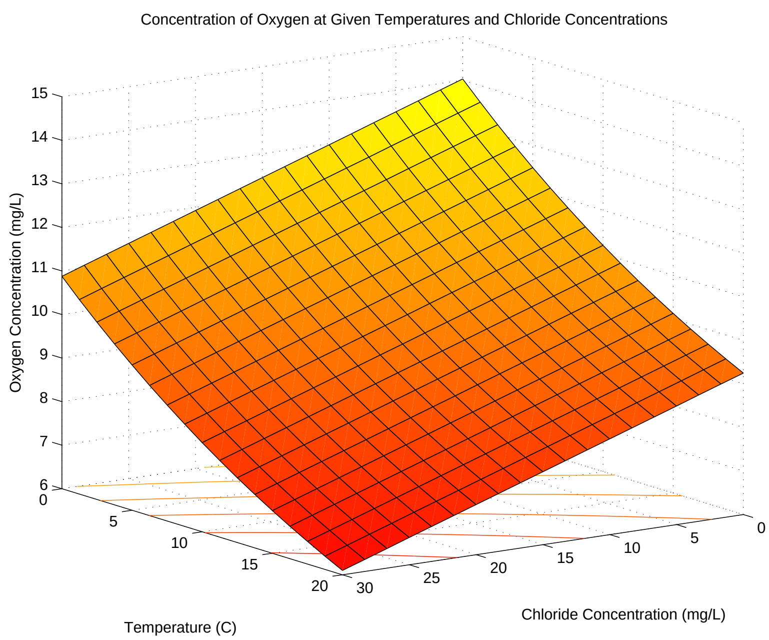

Figure 2: Chapra 15.7

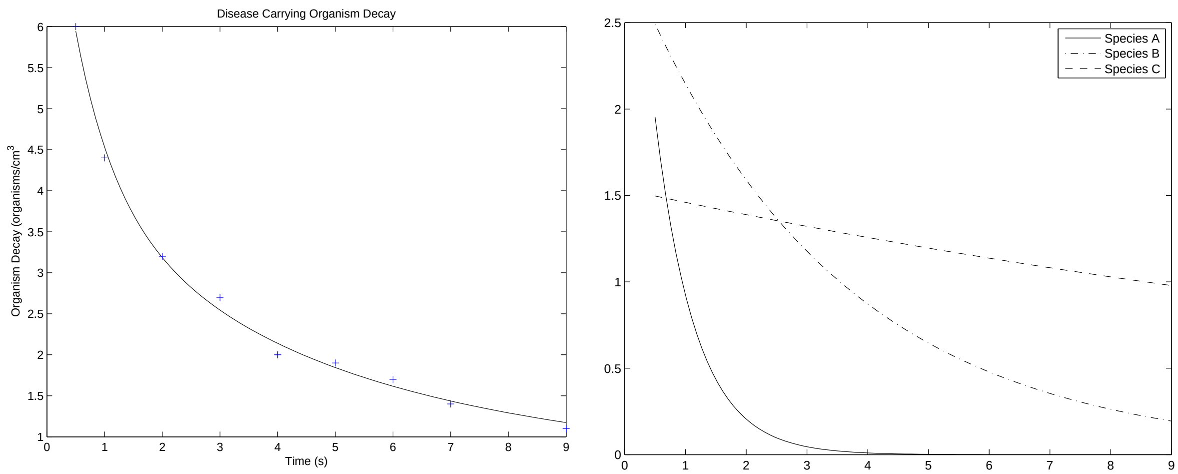

Figure 3: Chapra 15.10

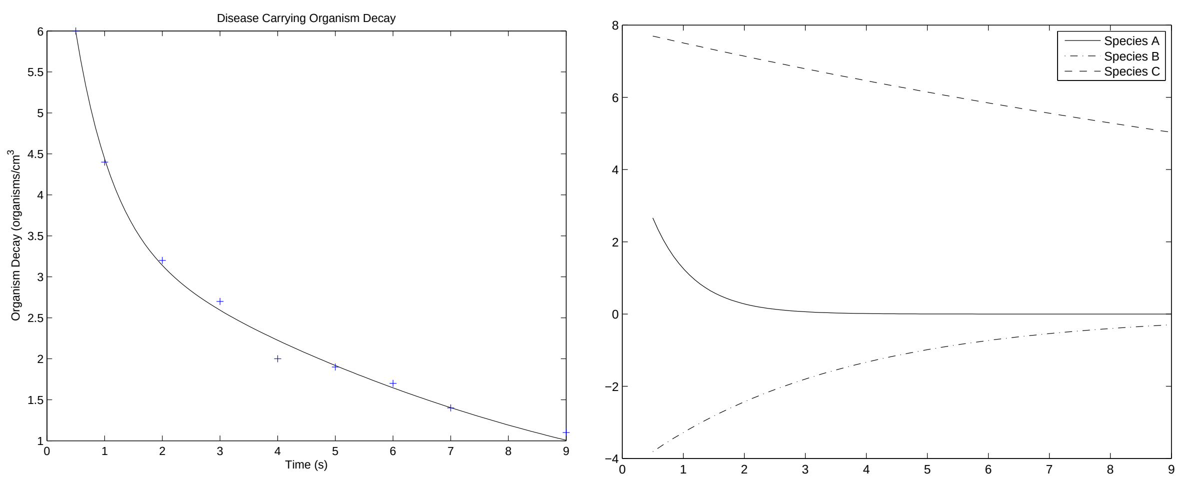

Figure 4: Chapra 15.10 Alternate

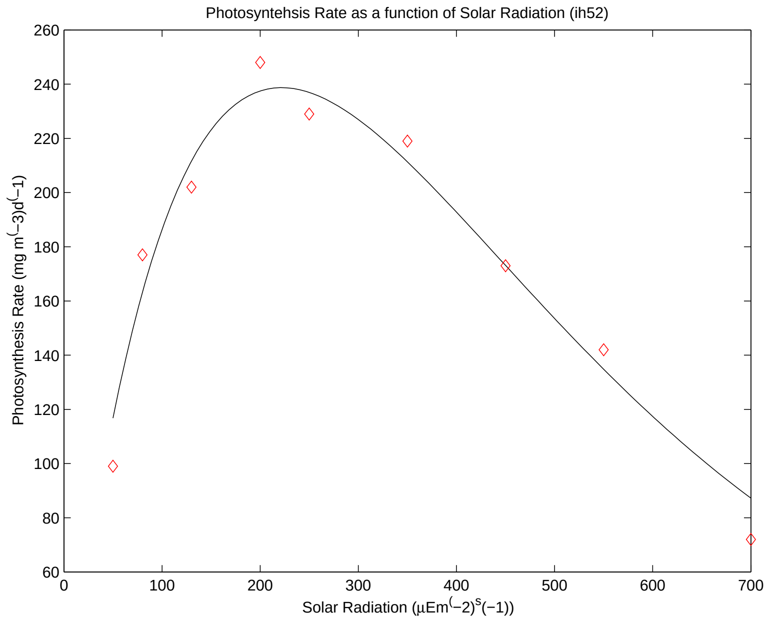

Figure 5: Chapra 15.11

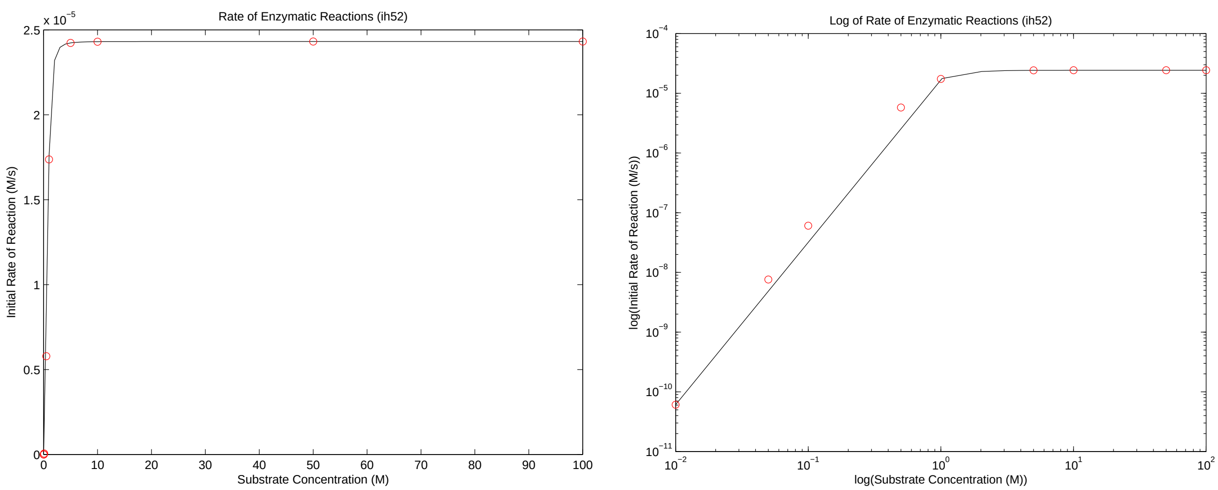

Figure 6: Chapra 15.14