

ENVE404: Environmental Modeling

Homework 4

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Instructors:

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Question 1)

a)

Script

```
clc
clear all
close all

v = [0.715 0.14 0.372 0.368 0.824 0.309 0.41 0.301 1.01 0.608];
d = [0.335 0.512 0.268 0.130 0.264 0.338 0.268 0.105 0.227 0.123];
w = [13.6 2.23 10.8 1.2 11.1 8.83 10 5 6.8 21.5];
L_y = [605 3.83 379 15.9 575 201 382 191 322 817];
D_x = [29.5 0.0771 9.83 0.652 31.9 4.91 11 3.72 24.6 20.8];

Pe = ((L_y.*v)./D_x)'; %Peclet number calculation
wd = (w./d)'; %mean depth ratio calculation
T = table(wd, Pe); %table of wd and Pe values
disp(T)
```

wd	Pe
40.597	14.664
4.3555	6.9546
40.299	14.343
9.2308	8.9742
42.045	14.853
26.124	12.649
37.313	14.238
47.619	15.455
29.956	13.22
174.8	23.882

```
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format short g
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d = [0.335 \ 0.512 \ 0.268 \ 0.130 \ 0.264 \ 0.338 \ 0.268 \ 0.105 \ 0.227 \ 0.123];
w = [13.6 \ 2.23 \ 10.8 \ 1.2 \ 11.1 \ 8.83 \ 10 \ 5 \ 6.8 \ 21.5];
L y = [605 \ 3.83 \ 379 \ 15.9 \ 575 \ 201 \ 382 \ 191 \ 322 \ 817];
D x = [29.5 \ 0.0771 \ 9.83 \ 0.652 \ 31.9 \ 4.91 \ 11 \ 3.72 \ 24.6 \ 20.8];
Pe = ((L_y.*v)./D_x)'; %Peclet number calculation
wd = (w./d)'; %mean depth ratio calculation
%Using the generalized least square method
Z = [ones(size(Pe)) log(wd)];
a = (Z'*Z) \setminus (Z'*log(wd));
fprintf('Alpha:%8.4f\n', a(1))
fprintf('Beta:%8.4f\n', a(2))
PeE = a(1) + a(2) * log(wd); %Pe estimates calculation
dif = Pe - PeE; %difference between calculated and estimated Pe values
MQE = sqrt(sum(dif.*dif))/10; %MQE calculation
fprintf('Mean Quadratic Error:%8.4f\n', MQE)
```

Results

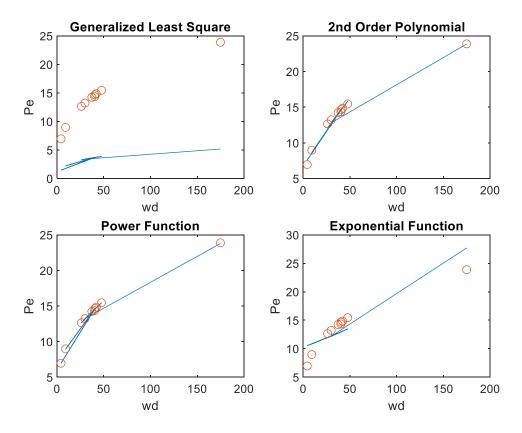
Alpha: 0.0000 Beta: 1.0000

Mean Quadratic Error: 3.4852

```
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d = [0.335 0.512 0.268 0.130 0.264 0.338 0.268 0.105 0.227 0.123];
w = [13.6 \ 2.23 \ 10.8 \ 1.2 \ 11.1 \ 8.83 \ 10 \ 5 \ 6.8 \ 21.5];
L y = [605 \ 3.83 \ 379 \ 15.9 \ 575 \ 201 \ 382 \ 191 \ 322 \ 817];
\overline{D} x = [29.5 0.0771 9.83 0.652 31.9 4.91 11 3.72 24.6 20.8];
Pe = ((L y.*v)./D x)'; %Peclet number calculation
wd = (w./d)'; %mean depth ratio calculation
%Finding coefficients for 2nd order polynomial
pPoly=polyfit (wd, Pe, 2);
%calculating MQE for 2nd order polynomial
PeE1 = pPoly(1).*(wd.^2)+pPoly(2).*wd+pPoly(3);
dif1 = Pe - (PeE1);
MQE_Poly = sqrt(sum(dif1.*dif1))/10;
fprintf('MQE for 2nd Order Polynomial:%8.4f\n', MQE_Poly)
%Finding coefficients for power function
pPow=polyfit(log(wd),log(Pe),1);
%calculating MQE for power function
PeE2 = exp(pPow(2)).*((wd).^pPow(1));
dif2 = Pe - (PeE2);
MQE_Pow = sqrt(sum(dif2.*dif2))/10;
fprintf('MQE for Power function:%8.4f\n', MQE_Pow)
%Finding coefficients for exponential function
pExp=polyfit(wd,log(Pe),1);
%calculating MQE for exponential function
PeE3 = exp(pExp(2)).*exp(pExp(1).*wd);
dif3 = Pe - (PeE3);
MQE_Exp = sqrt(sum(dif3.*dif3))/10;
fprintf('MQE for Exponential function:%8.4f\n', MQE Exp)
```

```
MQE for 2nd Order Polynomial: 0.1113
MQE for Power function: 0.0280
MQE for Exponential function: 0.6865
```

```
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d = [0.335 \ 0.512 \ 0.268 \ 0.130 \ 0.264 \ 0.338 \ 0.268 \ 0.105 \ 0.227 \ 0.123];
W = [13.6 \ 2.23 \ 10.8 \ 1.2 \ 11.1 \ 8.83 \ 10 \ 5 \ 6.8 \ 21.5];
L y = [605 \ 3.83 \ 379 \ 15.9 \ 575 \ 201 \ 382 \ 191 \ 322 \ 817];
D x = [29.5 \ 0.0771 \ 9.83 \ 0.652 \ 31.9 \ 4.91 \ 11 \ 3.72 \ 24.6 \ 20.8];
\label{eq:pe} \texttt{Pe} \; = \; (\; (\texttt{L}\_\texttt{y}. * \texttt{v}) \, . \, / \texttt{D}\_\texttt{x}) \; '; \quad \text{\$Peclet number calculation}
wd = (w./d)'; %mean depth ratio calculation
%Using the generalized least square method for Pe estimates
Z = [ones(size(Pe)) log(wd)];
E = (Z'*Z) \setminus (Z'*log(wd));
PeE = E(2) * log(wd) + E(1);
%Using the 2nd order polynomial for Pe estimates
pPoly=polyfit (wd, Pe, 2);
PeE1 = pPoly(1).*(wd.^2)+pPoly(2).*wd+pPoly(3);
%Using the power function for Pe estimates
pPow=polyfit(log(wd),log(Pe),1);
PeE2 = exp(pPow(2)).*((wd).^pPow(1));
%Using the exponential for Pe estimates
pExp=polyfit(wd,log(Pe),1);
PeE3 = exp(pExp(2)).*exp(pExp(1).*wd);
subplot(2,2,1)
plot(wd, PeE, '-', wd, Pe, 'o'); %plotting for generalized least square method
title('Generalized Least Square')
xlabel('wd')
ylabel('Pe')
subplot(2,2,2)
plot(wd, PeE1, '-', wd, Pe, 'o');
                                   %plotting for 2nd order polynomial
title('2nd Order Polynomial')
xlabel('wd')
ylabel('Pe')
subplot(2,2,3)
plot(wd, PeE2, '-', wd, Pe, 'o'); %plotting for power function
title('Power Function')
xlabel('wd')
ylabel('Pe')
subplot(2,2,4)
plot(wd, PeE3, '-', wd, Pe, 'o');
                                    %plotting for exponential function
title('Exponential Function')
xlabel('wd')
ylabel('Pe')
```



```
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d = [0.335 \ 0.512 \ 0.268 \ 0.130 \ 0.264 \ 0.338 \ 0.268 \ 0.105 \ 0.227 \ 0.123];
W = [13.6 \ 2.23 \ 10.8 \ 1.2 \ 11.1 \ 8.83 \ 10 \ 5 \ 6.8 \ 21.5];
L y = [605 3.83 379 15.9 575 201 382 191 322 817];
Dx = [29.5 \ 0.0771 \ 9.83 \ 0.652 \ 31.9 \ 4.91 \ 11 \ 3.72 \ 24.6 \ 20.8];
Pe = ((L y.*v)./D x)'; %Peclet number calculation
wd = (w./d)'; %mean depth ratio calculation
%Finding coefficients for Generalized Least Square method
Z = [ones(size(Pe)) log(wd)];
a = (Z'*Z) \setminus (Z'*log(wd));
%calculating MQE for Generalized Least Square method
PeE = a(2) * log(wd);
dif = Pe - PeE;
MQE = sqrt(sum(dif.*dif))/10;
%Finding coefficients for 2nd order polynomial
pPoly=polyfit (wd, Pe, 2);
%calculating MQE for 2nd order polynomial
PeE1 = pPoly(1).*(wd.^2)+pPoly(2).*wd+pPoly(3);
dif1 = Pe - (PeE1);
MQE_Poly = sqrt(sum(dif1.*dif1))/10;
%Finding coefficients for power function
pPow=polyfit(log(wd),log(Pe),1);
%calculating MQE for power function
PeE2 = exp(pPow(2)).*((wd).^pPow(1));
dif2 = Pe - (PeE2);
MQE Pow = sqrt(sum(dif2.*dif2))/10;
%Finding coefficients for exponential function
pExp=polyfit(wd,log(Pe),1);
%calculating MQE for exponential function
PeE3 = exp(pExp(2)).*exp(pExp(1).*wd);
dif3 = Pe - (PeE3);
MQE_Exp = sqrt(sum(dif3.*dif3))/10;
%creating table for methods and their MQEs
MQEval = [MQE, MQE_Poly, MQE_Pow, MQE_Exp];
fprintf('Method
                                    MQE Calculated\n')
fprintf('Generalized Least Square %8.4f\n', MQEval(1))
fprintf('2nd Order Polynomial
                                    %8.4f\n',MQEval(2))
fprintf('Power function
                                    %8.4f\n',MQEval(3))
fprintf('Exponential function
                                   %8.4f\n',MQEval(4))
%finding out the best fit based on MQEs
if MQEval(1) == min(MQEval)
    fprintf('\nGeneralized Least Square Method is the best fit\n')
elseif MQEval(2) == min(MQEval)
        fprintf('\n2nd oder Polynomial function is the best fit\n')
elseif MQEval(3) == min(MQEval)
   fprintf('\nPower function is the best fit\n')
elseif MQEval(4) == min(MQEval)
        fprintf('\nExponential function is the best fit\n')
```

Results

```
Method MQE Calculated
Generalized Least Square 3.4852
2nd Order Polynomial 0.1113
Power function 0.0280
Exponential function 0.6865

Power function is the best fit
```

Question 2)

a)

Function

```
%function for optimizing longitudinal dispersion coefficient
function f = fSSR(D,t,C_50)
v = 0.5;
C_0 = 80;
x = 50;

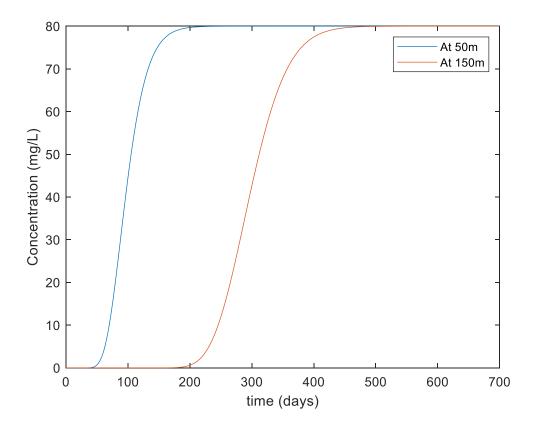
C = (C_0/2).*(erfc((x-v.*t)./(2*sqrt(D.*t)))+exp((v.*x)/D)*...
        erfc((x+v.*t)./(2*sqrt(D.*t))));
f = sum(sqrt(C_50-C));
end
```

Script

```
clear all
close all
clc
v = 0.5;
C_0 = 80;
x = 50;
t = 0:100:700;
C 50 = [0,40,59.6 69 73 76 77.5 78.5];
%using fuction fSSR.m to calculate D
D = fminsearch(@fSSR,1,[],t,C_50);
fprintf('The longitudinal dispersion coefficient(m^2/day): 88.4f\n',D)
%using D value to calculate C values at 50m
\texttt{C} \; = \; (\texttt{C}\_\texttt{0/2}) \, . \, \star \, (\texttt{erfc} \, (\, (\texttt{x-v.*t}) \, . \, / \, (2 \, \star \, \texttt{sqrt} \, (\texttt{D.*t}) \, ) \, ) \, + \texttt{exp} \, (\, (\texttt{v.*x}) \, / \, \texttt{D}) \, \star \, \ldots \,
      (erfc((x+v.*t)./(2*sqrt(D.*t))));
calculating MQE using given and calculated C values at 50m
dif = C-C 50;
MQE = sqrt(sum(dif.*dif))/length(t);
fprintf('MQE: %8.4f\n',MQE)
```

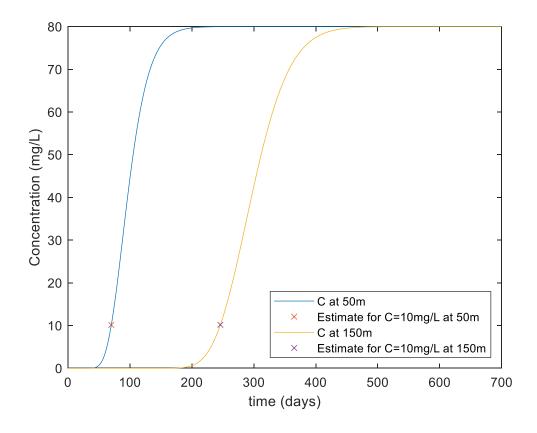
```
The longitudinal dispersion coefficient(m^2/day): 1.0000 MQE: 3.1064
```

```
clear all
close all
clc
v = 0.5;
C 0 = 80;
t = 0:700;
D = 1; %calculated dispersion coefficient
x = [50 \ 150];
%plotting C values at 50m and 150m
for i = 1:length(x)
   for j = 1:length(t)
   erfc((x(i)+v.*t(j))./(2*sqrt(D.*t(j)))));
   end
   plot(t,C(i,:))
   xlabel('time (days)')
   ylabel('Concentration (mg/L)')
   hold on
legend('At 50m','At 150m')
```



```
clear all
close all
clc
v = 0.5;
C_0 = 80;
t = 0:700;
D = 1; %calculated dispersion coefficient
x = [50 \ 150];
for i = 1:length(x)
    %plotting C values at 50m and 150m
    for j = 1:length(t)
    C(i,j) = (C 0/2).*(erfc((x(i)-v.*t(j))./(2*sqrt(D.*t(j)))))+exp((v.*x(i)/D))*...
    erfc((x(i)+v.*t(j))./(2*sqrt(D.*t(j)))));
    plot(t,C(i,:))
   xlabel('time (days)')
    ylabel('Concentration (mg/L)')
    hold on
    %estimating time for C to reach 10\,\mathrm{mg/L} at 50\mathrm{m} and 150\mathrm{m}
    diff = abs(C-10);
    for h = 1:length(t)
        if diff(i,h) == min(diff(i,:))
            %plotting C values closest to 10mg/L
            plot(t(h),C(i,h),'x')
            fprintf('Time for concentration to reach 10mg/L at %dm: %d days\n'...
                ,x(i), t(h))
        end
    end
end
legend('C at 50m', 'Estimate for C=10mg/L at 50m', 'C at 150m',...
'Estimate for C=10mg/L at 150m', 'Location', 'southeast')
```

```
Time for concentration to reach 10\,\mathrm{mg/L} at 50\mathrm{m}: 70 days Time for concentration to reach 10\,\mathrm{mg/L} at 150\mathrm{m}: 246 days
```



```
clear all
close all
clc
v = 0.5;
C 0 = 80;
t = 0:700;
D = 1; %calculated dispersion coefficient
x = [50 \ 150];
for i = 1:length(x)
    %plotting C values at 50m and 150m
    for j = 1:length(t)
    \texttt{C(i,j)} \ = \ (\texttt{C_0/2}) \cdot (\texttt{erfc((x(i)-v.*t(j))./(2*sqrt(D.*t(j))))}) + \texttt{exp((v.*x(i)/D))*...}
    erfc((x(i)+v.*t(j))./(2*sqrt(D.*t(j)))));
    plot(t,C(i,:))
    xlabel('time (days)')
    ylabel('Concentration (mg/L)')
    hold on
    %estimating time for C to reach steadt state at 50m and 150m
    for h = 1:length(t)
        if round(C(i,h),4) == round(max(C(i,:)),4)
            %plotting steady state C values
            plot(t(h),C(i,h),'x')
             fprintf('Time for concentration to reach steady state at %dm: %d days\n'...
                ,x(i),t(h))
            break
        end
    end
end
legend('C at 50m', 'Estimate for steady state C at 50m', 'C at 150m',...
'Estimate for steady state C at 150m', 'Location', 'southeast')
```

```
Time for concentration to reach steady state at 50m: 347 days Time for concentration to reach steady state at 150m: 641 days
```

