
```
%{
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Subject: Assignment2 Q8
%}

function Prob8()
clear all % Clear stored variables
clc % Clear the screen
close all % Close all previously created plots

% Given values of K1 and K2 in case a
K11 = 0.1071;
K21 = 0.01493;

% Given initial concentrations of components
NoCO21 = 0.3333333333;
NoO21 = 0.3333333333;
NoN21 = 0.3333333333;
NoCO1 = 0;
NoNO1 = 0;

% Given values of K1 and K2 in case a
K12 = 0.1071;
K22 = 0.01493;

% Given initial concentrations of components
NoCO22 = 2;
NoO22 = 0.3333333333;
NoN22 = 0.3333333333;
NoCO2 = 0;
NoNO2 = 0;
E = [0.5; 0.5];

%Calling functioneval1 for case a
fun1 = @(E) eval1 (E, K11, K21, NoCO21, NoO21, NoN21, NoCO1, NoNO1);
fun1(E);
%Calling functioneval1 for case b
fun2 = @(E) eval1(E, K12, K22, NoCO22, NoO22, NoN22, NoCO2, NoNO2);
fun2(E);
options = optimoptions('fsolve','Display','iter');
[Ea] = fsolve(fun1, E, options);
[Eb] = fsolve(fun2, E, options);

disp('For case a the extent of reaction is (E1 and E2)')
Ea
disp('For case b the extent of reaction is (E1 and E2)')
Eb
end
```

```

function func = eval1(E, K1, K2, NoCO2, NoO2, NoN2, NoCO, NoNO)

%Defining the functions which will be returned when called
func(1) = (((NoCO + 2*E(1))^2)*(NoO2 - E(2) + E(1)))/(((NoCO2 -
2*E(1))^2)*(NoCO2 + NoCO + NoO2 + NoN2 + NoNO + E(1)))-K1;
func(2) = (((NoNO + 2*E(2))^2)/((NoO2 + E(1) - E(2))*(NoN2 - E(2))))-
K2;

end

```

<i>Trust-region</i>			<i>Norm of</i>	<i>First-order</i>
<i>Iteration</i>	<i>Func-count</i>	<i>f(x)</i>	<i>step</i>	<i>optimality</i>
<i>radius</i>				
0	3	324.692		973
1				
1	6	143.763	0.536168	365
1				
2	9	45.7472	1	69.4
1				
3	12	11.7483	1	11.5
1				
4	15	3.02318	1	0.722
1				
5	18	0.668911	1	0.0928
1				
6	21	0.618679	2.5	0.536
2.5				
7	22	0.618679	6.25	0.536
6.25				
8	23	0.618679	1.5625	0.536
1.56				
9	26	0.599584	0.390625	0.104
0.391				
10	27	0.599584	0.390625	0.104
0.391				
11	30	0.598522	0.0976563	0.109
0.0977				
12	33	0.598135	0.0976563	0.0643
0.0977				
13	34	0.598135	0.0976563	0.0643
0.0977				
14	37	0.597965	0.0244141	0.0578
0.0244				
15	40	0.597797	0.0244141	0.0258
0.0244				
16	41	0.597797	0.0244141	0.0258
0.0244				
17	44	0.597779	0.00610352	0.0193
0.0061				
18	47	0.597764	0.00610352	0.0125
0.0061				

19	50	0.597763	0.00610352	0.00936
0.0061				
20	53	0.597758	0.00610352	0.00678
0.0061				
21	54	0.597758	0.00610352	0.00678
0.0061				
22	57	0.597757	0.00152588	0.0047
0.00153				
23	60	0.597756	0.00152588	0.00321
0.00153				
24	63	0.597755	0.00152588	0.00187
0.00153				
25	66	0.597755	0.00152588	0.000959
0.00153				
26	69	0.597755	0.00152588	0.000392
0.00153				
27	70	0.597755	0.00152588	0.000392
0.00153				
28	73	0.597755	0.00038147	0.000195
0.000381				
29	74	0.597755	0.00038147	0.000195
0.000381				
30	77	0.597755	9.53674e-05	0.00014
9.54e-05				
31	80	0.597755	9.53674e-05	0.000105
9.54e-05				
32	81	0.597755	9.53674e-05	0.000105
9.54e-05				
33	84	0.597755	2.38419e-05	7.12e-05
2.38e-05				
34	87	0.597755	2.38419e-05	4.94e-05
2.38e-05				
35	90	0.597755	2.38419e-05	3.55e-05
2.38e-05				
36	93	0.597755	2.38419e-05	2.66e-05
2.38e-05				
37	96	0.597755	2.38419e-05	2.08e-05
2.38e-05				
38	97	0.597755	2.38419e-05	2.08e-05
2.38e-05				
39	100	0.597755	5.96046e-06	1.43e-05
5.96e-06				
40	103	0.597755	5.96046e-06	8.33e-06
5.96e-06				
41	106	0.597755	5.96046e-06	4.46e-06
5.96e-06				
42	109	0.597755	5.96046e-06	1.98e-06
5.96e-06				
43	110	0.597755	5.96046e-06	1.98e-06
5.96e-06				
44	113	0.597755	1.49012e-06	1.05e-06
1.49e-06				
45	114	0.597755	1.49012e-06	1.05e-06
1.49e-06				

46	117	0.597755	3.72529e-07	7.37e-07
3.73e-07				

No solution found.

fsolve stopped because the problem appears regular as measured by the gradient,
but the vector of function values is not near zero as measured by the default value of the function tolerance.

Trust-region Iteration	Func-count	f(x)	Norm of step	First-order optimality
radius				
0	3	324.538		973
1				
1	6	0.882078	1	1.73
1				
2	9	0.0052727	0.497895	0.114
2.5				
3	10	0.0052727	0.135749	0.114
2.5				
4	13	0.000770041	0.0339372	0.0281
0.0339				
5	14	0.000770041	0.0848431	0.0281
0.0848				
6	17	0.000162829	0.0212108	0.00541
0.0212				
7	18	0.000162829	0.0312042	0.00541
0.053				
8	21	7.64897e-05	0.00780104	0.00573
0.0078				
9	24	1.04821e-05	0.0127548	0.00405
0.0195				
10	27	2.60839e-08	0.00262437	0.000182
0.0195				
11	30	2.34452e-13	0.000145191	5.43e-07
0.0195				

Equation solved.

fsolve completed because the vector of function values is near zero as measured by the default value of the function tolerance, and the problem appears regular as measured by the gradient.

For case a the extent of reaction is (E1 and E2)

Ea =

1.4991
0.1141

For case b the extent of reaction is (E1 and E2)

Eb =

0.4050
0.0284

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