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Here I have shown the code to solve question 4 of assignment:

We need to solve simultenous non-linear equations here.

Contents

Defining Constants :

Here we will define the constant terms of the code:

```
Kc1 = 1.06 ; Kc2 = 2.63 ; Kc3 = 5 ;
CA0 = 1.5 ; CB0 = 1.5 ;
```

Defining the Reactions and Extent of Reactions :

```
%
% For future references:
%
% Index corresponding to species are : A-1,B-2,C-3,D-4,X-5,Y-6,Z-7
% Uncomment according to use
n = 7 ;% input('Enter number of Species : ') ; % Enter Number of Species
m = 3 ;% input('Enter Number of Reactions :') ; % Enter Number of Reactions
% The reaction is given as :
%
% A + B --> C + D
% B + C --> X + Y
% A + X --> Z
%
ICM = zeros(n,1) ; % Initial Concentration Matrix
ICM(1) = CA0 ; ICM(2) = CB0 ;
CM = zeros(n,1) ;   % Concentration Matrix
```

Defining the function to be solved :

```
conc = @(C) [ (C(3)*C(4))-Kc1*(C(1)*C(2)) ;
              (C(5)*C(6))-Kc2*(C(2)*C(3)) ;
              (C(7))-Kc3*(C(3)*C(2)) ;
               C(1) - CA0 + C(4) + C(7) ;
               C(2) - CB0 + C(4) + C(6) ;
               C(3) - C(4) + C(6) ;
               C(6) - C(5) - C(7) ; ];
```

Solving the function with different guess values

Here we will see how can we solve the above defined function for different guess values as given in the question :

```
%The first guess:
conc0_1 = 0.001*(ones(size(CM))) ;
conc0_1([4,5,7]) = [0 0 0];
conc_1 = fsolve(conc,conc0_1);
% Second Guess :
conc0_2 = 0.001*(ones(size(CM))) ;
conc0_2([4,5,7]) = [1 1 1];
conc_2 = fsolve(conc,conc0_2);
% Third Guess :
conc0_3 = 0.001*(ones(size(CM))) ;
conc0_3([4,5,7]) = [10 10 10];
conc_3 = fsolve(conc,conc0_3);
```

```
Equation solved.

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


Equation solved.

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Equation solved.
```

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

Displaying Results

```
species = ['A';'B';'C';'D';'X';'Y';'Z'];
ind = 1:n;
T = table(ind',species,ICM,conc_1,conc_2,conc_3,'VariableNames',{'Sr.No','Species','Initial Concentration','First Guess','Second Guess','Third Guess'});
disp(T); disp(['Sum of Conc of species = ',num2str(sum(conc_3))])
```

Sr.No	Species	Initial Concentration	First Guess	Second Guess	Third Guess
1	A	1.5	0.52131	0.52131	0.52131
2	B	1.5	0.2597	0.2597	0.2597
3	C	0	0.19936	0.19936	0.19936
4	D	0	0.71983	0.71983	0.71983
5	X	0	0.26161	0.26161	0.26161
6	Y	0	0.52047	0.52047	0.52047
7	Z	0	0.25886	0.25886	0.25886

```
Sum of Conc of species = 2.7411
```

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