CAPE Laboratory Assignment-3

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Q.1

Problem Statement

1. Consider an ideal plug flow reactor (PFR) where the following reaction takes place:

   A → Products

   The model of the system and kinetic parameters are given as

$$u\frac{dC_A}{dz} = -\frac{kC_A}{\sqrt{1+K_rC_A^2}}$$

$$k = 2\,\mathrm{s}^{-1}, \quad K_r = 1\,\mathrm{mol}^2/\mathrm{m}^6$$

   The velocity u is given by, $u = Q/A$ where Q is inlet volumetric flowrate and A is the area of cross-section of the PFR. Consider a PFR with length z = 1m, A = 0.40 m^2, Q = 0.2 m^3/s, C_{A0} = 1 mol/m^3. Determine and PLOT the concentration C_A and conversion (X_A) along the length (z) of the PFR.

   (a) Implement 4th order RK method to solve this.

   (b) Compare your results with that obtained using MATLAB function `ode45`

MATLAB Code

4th order Runge Kutta method

(divided the length span in 101 points)

```
global u k Kr
k = 2; % s^-1
```

```
Kr = 1; % mol^2 m^-6
z = 1; % length of PFR
A = 0.4; % m^2
Q = 0.2; % m^3 s^-1
CA0 = 1; % mol m^-3
u = Q/A; % velocity
h = 0.01;
l = 0:h:z;
CA(1) = CA0;

for i=1:(z/h)
k1 = fun(CA(i));
k2 = fun(CA(i)+(h/2)*k1);
k3 = fun(CA(i)+(h/2)*k2);
k4 = fun(CA(i)+h*k3);
CA(i+1) = CA(i) + (h/6)*(k1+2*k2+2*k3+k4);
end

XA = (CA0 - CA)/CA0;
plot(l,CA,'-o','LineWidth',2);
hold on;
plot(l, XA,'-x','LineWidth',2);
legend('CA','XA');

function s = fun(CA)
global u k Kr
s = -(1/u)*k*CA/sqrt(1+Kr*(CA^2));
end
```

ode45 method

(length span division is default)

```
global u k Kr
k = 2; % s^-1
Kr = 1; % mol^2 m^-6
z = 1; % length of PFR
A = 0.4; % m^2
Q = 0.2; % m^3 s^-1
CA0 = 1; % mol m^-3
u = Q/A; % velocity
l = [0 z];

[length,CA_sol] = ode45(@(l,CA) -
(1/u)*k*CA/sqrt(1+Kr*(CA^2)),l,CA0);
XA = (CA0 - CA_sol)/CA0;
plot(length,CA_sol,'-o','LineWidth',2);
```

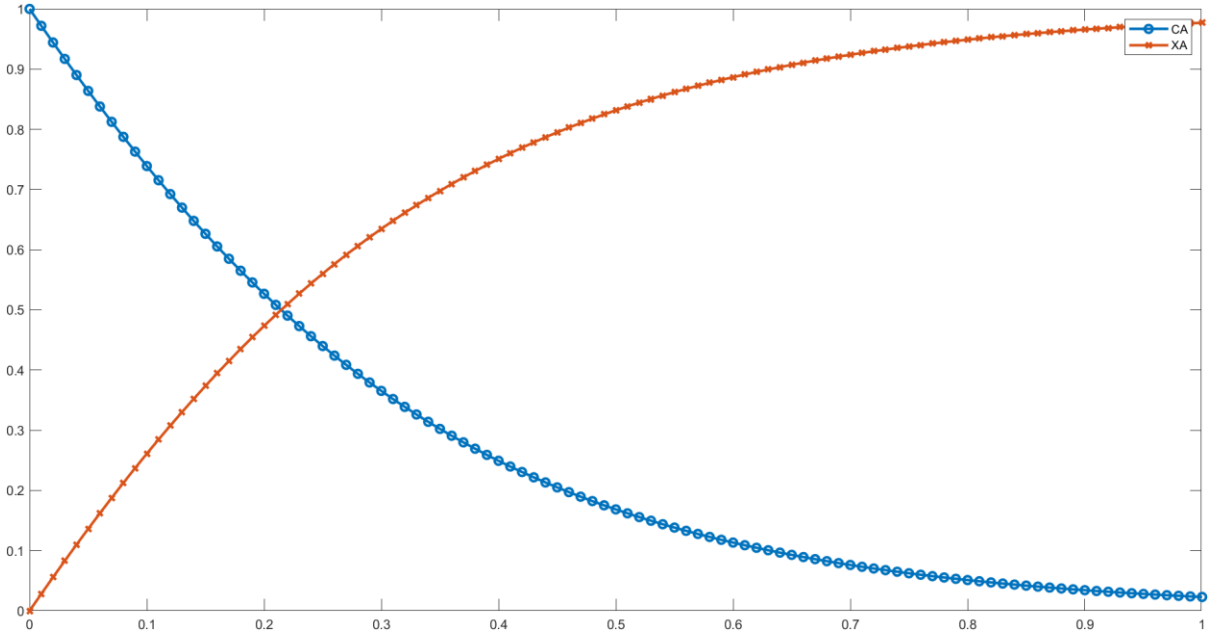
```
hold on;
plot(length, XA,'-x','LineWidth',2);
legend('CA','XA');
```

Results

Length (z)	C_A	X_A
0	1	0
0.0100000000000000	0.971917607284530	0.0280823927154701
0.0200000000000000	0.944246419995474	0.0557535800045265
0.0300000000000000	0.916997436245865	0.0830025637541348
0.0400000000000000	0.890181370933788	0.109818629066212
0.0500000000000000	0.863808591438300	0.136191408561700
0.0600000000000000	0.837889052348865	0.162110947651135
0.0700000000000000	0.812432230089295	0.187567769910705
0.0800000000000000	0.787447058368295	0.212552941631705
0.0900000000000000	0.762941865438657	0.237058134561343
0.100000000000000	0.738924314172167	0.261075685827833
0.110000000000000	0.715401345954232	0.284598654045768
0.120000000000000	0.692379129369242	0.307620870630759
0.130000000000000	0.669863014584233	0.330136985415767
0.140000000000000	0.647857494245361	0.352142505754639
0.150000000000000	0.626366171581560	0.373633828418440
0.160000000000000	0.605391736266426	0.394608263733574
0.170000000000000	0.584935948427994	0.415064051572006
0.180000000000000	0.564999631022737	0.435000368977263
0.190000000000000	0.545582670611612	0.454417329388389
0.200000000000000	0.526684026399109	0.473315973600891
0.210000000000000	0.508301747227783	0.491698252772217
0.220000000000000	0.490432996066629	0.509567003933371
0.230000000000000	0.473074081397061	0.526925918602939
0.240000000000000	0.456220494789070	0.543779505210930
0.250000000000000	0.439866953874825	0.560133046125175
0.260000000000000	0.424007449868937	0.575992550131063
0.270000000000000	0.408635298753421	0.591364701246579
0.280000000000000	0.393743195239999	0.606256804760001
0.290000000000000	0.379323268640321	0.620676731359679
0.300000000000000	0.365367139812924	0.634632860187076
0.310000000000000	0.351865978410875	0.648134021589125
0.320000000000000	0.338810559722111	0.661189440277889
0.330000000000000	0.326191320471886	0.673808679528114
0.340000000000000	0.313998413039748	0.686001586960252
0.350000000000000	0.302221757628794	0.697778242371206
0.360000000000000	0.290851092009854	0.709148907990146
0.370000000000000	0.279876018545160	0.720123981454840
0.380000000000000	0.269286048273213	0.730713951726787
0.390000000000000	0.259070641907566	0.740929358092434
0.400000000000000	0.249219247666050	0.750780752333950
0.410000000000000	0.239721335903206	0.760278664096794
0.420000000000000	0.230566430567063	0.769433569432937

0.430000000000000	0.221744137542065	0.778255862457935
0.440000000000000	0.213244169973243	0.786755830026757
0.450000000000000	0.205056370693092	0.794943629306908
0.460000000000000	0.197170731892744	0.802829268107256
0.470000000000000	0.189577412193453	0.810422587806547
0.480000000000000	0.182266751283998	0.817733248716002
0.490000000000000	0.175229282294845	0.824770717705155
0.500000000000000	0.168455742081690	0.831544257918310
0.510000000000000	0.161937079589738	0.838062920410262
0.520000000000000	0.155664462466452	0.844335537533548
0.530000000000000	0.149629282085070	0.850370717914930
0.540000000000000	0.143823157134238	0.856176842865763
0.550000000000000	0.138237935921213	0.861762064078787
0.560000000000000	0.132865697527500	0.867134302472500
0.570000000000000	0.127698751946725	0.872301248053275
0.580000000000000	0.122729639325389	0.877270360674611
0.590000000000000	0.117951128417959	0.882048871582041
0.600000000000000	0.113356214358697	0.886643785641303
0.610000000000000	0.108938115843920	0.891061884156080
0.620000000000000	0.104690271809936	0.895309728190065
0.630000000000000	0.100606337683945	0.899393662316055
0.640000000000000	0.0966801812776703	0.903319818722330
0.650000000000000	0.0929058783864113	0.907094121613589
0.660000000000000	0.0892777081496815	0.910722291850319
0.670000000000000	0.0857901482235074	0.914209851776493
0.680000000000000	0.0824378698088823	0.917562130191118
0.690000000000000	0.0792157325757441	0.920784267424256
0.700000000000000	0.0761187795171693	0.923881220482831
0.710000000000000	0.0731422317642193	0.926857768235781
0.720000000000000	0.0702814833880186	0.929718516611981
0.730000000000000	0.0675320962121598	0.932467903787840
0.740000000000000	0.0648897946553905	0.935110205344610
0.750000000000000	0.0623504606217211	0.937649539378279
0.760000000000000	0.0599101284525659	0.940089871547434
0.770000000000000	0.0575649799532766	0.942435020046723
0.780000000000000	0.0553113395044226	0.944688660495577
0.790000000000000	0.0531456692663861	0.946854330733614
0.800000000000000	0.0510645644842639	0.948935435515736
0.810000000000000	0.0490647488986730	0.950935251101327
0.820000000000000	0.0471430702668295	0.952856929733171
0.830000000000000	0.0452964959971904	0.954703504002810
0.840000000000000	0.0435221089000092	0.956477891099991
0.850000000000000	0.0418171030553278	0.958182896944672
0.860000000000000	0.0401787797992187	0.959821220200781
0.870000000000000	0.0386045438284684	0.961395456171532
0.880000000000000	0.0370918994233636	0.962908100576636
0.890000000000000	0.0356384467877855	0.964361553212215
0.900000000000000	0.0342418785054278	0.965758121494572
0.910000000000000	0.0328999761106292	0.967100023889371
0.920000000000000	0.0316106067720316	0.968389393227968

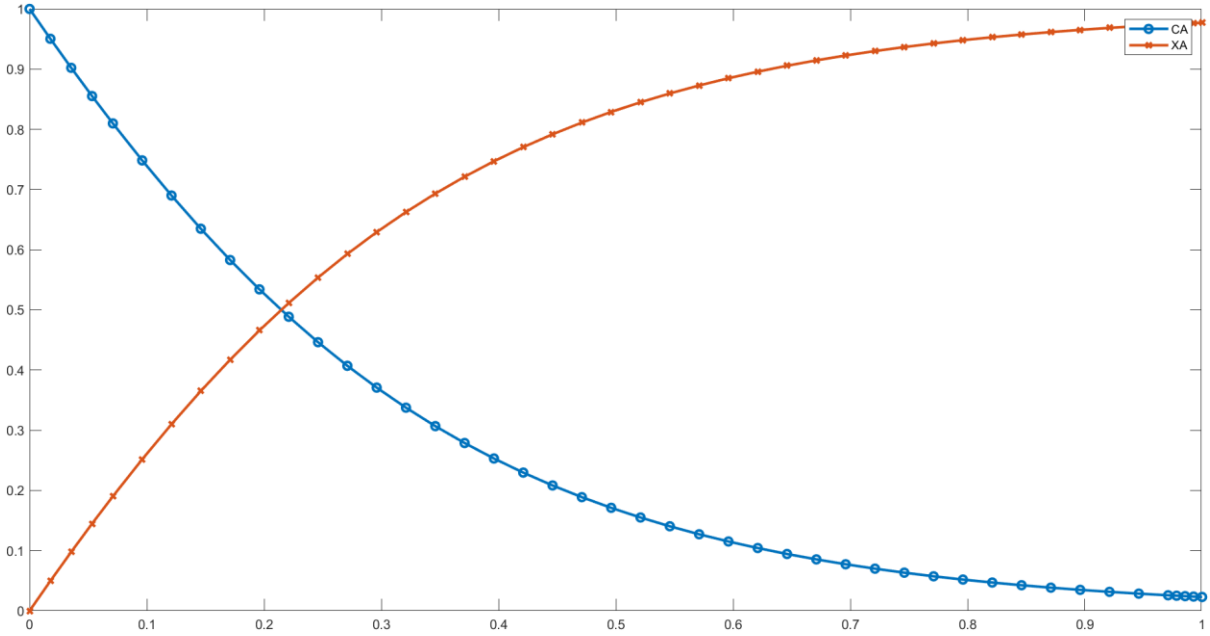
0.930000000000000	0.0303717200870520	0.969628279912948
0.940000000000000	0.0291813449849650	0.970818655015035
0.950000000000000	0.0280375867362457	0.971962413263754
0.960000000000000	0.0269386240657004	0.973061375934300
0.970000000000000	0.0258827063668235	0.974117293633177
0.980000000000000	0.0248681510147526	0.975131848985247
0.990000000000000	0.0238933407751439	0.976106659224856
1	0.0229567213062686	0.977043278693731



Plot using 4th order RK method

Length (z)	C_A	X_A
0	1	0
0.0177617192929090	0.950403608750618	0.0495963912493823
0.0355234385858181	0.902131509512916	0.0978684904870839
0.0532851578787271	0.855243212286957	0.144756787713043
0.0710468771716361	0.809794339239428	0.190205660760572
0.0960468771716361	0.748359464386972	0.251640535613028
0.121046877171636	0.689997686931994	0.310002313068006
0.146046877171636	0.634800259563848	0.365199740436152
0.171046877171636	0.582824502330490	0.417175497669510
0.196046877171636	0.534092811967884	0.465907188032116
0.221046877171636	0.488590992364694	0.511409007635306
0.246046877171636	0.446271455946184	0.553728544053816
0.271046877171636	0.407053856643349	0.592946143356651
0.296046877171636	0.370828902247703	0.629171097752297
0.321046877171636	0.337467865973380	0.662532134026620
0.346046877171636	0.306826967393335	0.693173032606665
0.371046877171636	0.278749474585508	0.721250525414492
0.396046877171636	0.253070160828099	0.746929839171902
0.421046877171636	0.229626045831646	0.770373954168354

0.446046877171636	0.208255547726260	0.791744452273740
0.471046877171636	0.188799076675269	0.811200923324731
0.496046877171636	0.171101877199258	0.828898122800742
0.521046877171636	0.155020591059849	0.844979408940151
0.546046877171636	0.140419441194940	0.859580558805060
0.571046877171636	0.127169614393238	0.872830385606762
0.596046877171636	0.115150793270969	0.884849206729031
0.621046877171636	0.104254472327842	0.895745527672158
0.646046877171636	0.0943799168824444	0.905620083117556
0.671046877171636	0.0854332426754375	0.914566757324563
0.696046877171636	0.0773282549762214	0.922671745023779
0.721046877171636	0.0699881386657237	0.930011861334276
0.746046877171636	0.0633422134676719	0.936657786532328
0.771046877171636	0.0573251281047494	0.942674871895251
0.796046877171636	0.0518773532958500	0.948122646704150
0.821046877171636	0.0469461184495158	0.953053881550484
0.846046877171636	0.0424830614957135	0.957516938504286
0.871046877171636	0.0384436262625342	0.961556373737466
0.896046877171636	0.0347873700762389	0.965212629923761
0.921046877171636	0.0314785271393216	0.968521472860678
0.946046877171636	0.0284843784471991	0.971515621552801
0.971046877171636	0.0257748282344645	0.974225171765536
0.978285157878727	0.0250394999086548	0.974960500091345
0.985523438585818	0.0243251370455199	0.975674862954480
0.992761719292909	0.0236311431152354	0.976368856884765
1	0.0229569380053415	0.977043061994659



Plot using ode45 method

Conclusion

Both methods took nearly the same time for computation because even the *ode45* algorithm involves the Runge-Kutta method. However, the conventional Runge-Kutta code occupied more memory because the length was spanned over a greater number of points. Therefore, more data points were considered in an effort to increase accuracy. Both the methods gave nearly same output values with slight deviation in higher decimal places which is not very significant. The conventional Runge-Kutta code might have lost some precision while having round-off errors in the computation procedure had we used the same number of points as *ode45*.

Q.2

Problem Statement

2. Consider the following system of ODE representing autocatalytic reactions. Consider the following initial conditions: $x = 1, y = 0, z = 0$.
   (a) Implement 4th order RK method to solve this.
   (b) Compare your results with that obtained using MATLAB function `ode15s`
   (c) Analyse your results.

$$\frac{dx}{dt} = -0.04x + 10^4 yz,$$
$$\frac{dy}{dt} = 0.04x - 10^4 yz - 3 \times 10^7 y^2,$$
$$\frac{dz}{dt} = 3 \times 10^7 y^2.$$

MATLAB Code

Multivariable 4th order Runge-Kutta method

(code with h = 0.01)

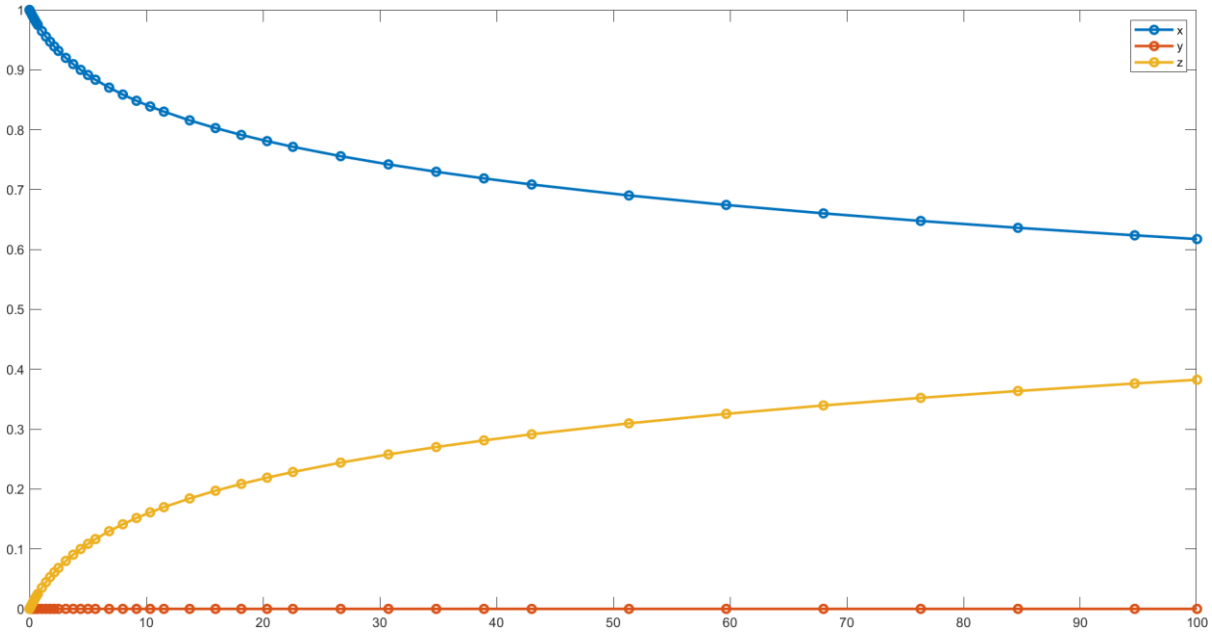
```
clear all;

x(1) = 1;
y(1) = 0;
z(1) = 0;
t = 0:0.01:100;
for i=1:10000
    k1 = func(t(i),x(i),y(i),z(i));
    k2 =
func(t(i)+0.005,x(i)+0.005*k1(1),y(i)+0.005*k1(2),z(i)+0.
005*k1(3));
    k3 =
func(t(i)+0.005,x(i)+0.005*k2(1),y(i)+0.005*k2(2),z(i)+0.
005*k2(3));
    k4 =
func(t(i)+0.01,x(i)+0.01*k3(1),y(i)+0.01*k3(2),z(i)+0.01*
k3(3));
    x(i+1) = x(i) + (1/6)*(k1(1)+2*k2(1)+2*k3(1)+k4(1));
    y(i+1) = y(i) + (1/6)*(k1(2)+2*k2(2)+2*k3(2)+k4(2));
    z(i+1) = z(i) + (1/6)*(k1(3)+2*k2(3)+2*k3(3)+k4(3));
end
t = t';
```

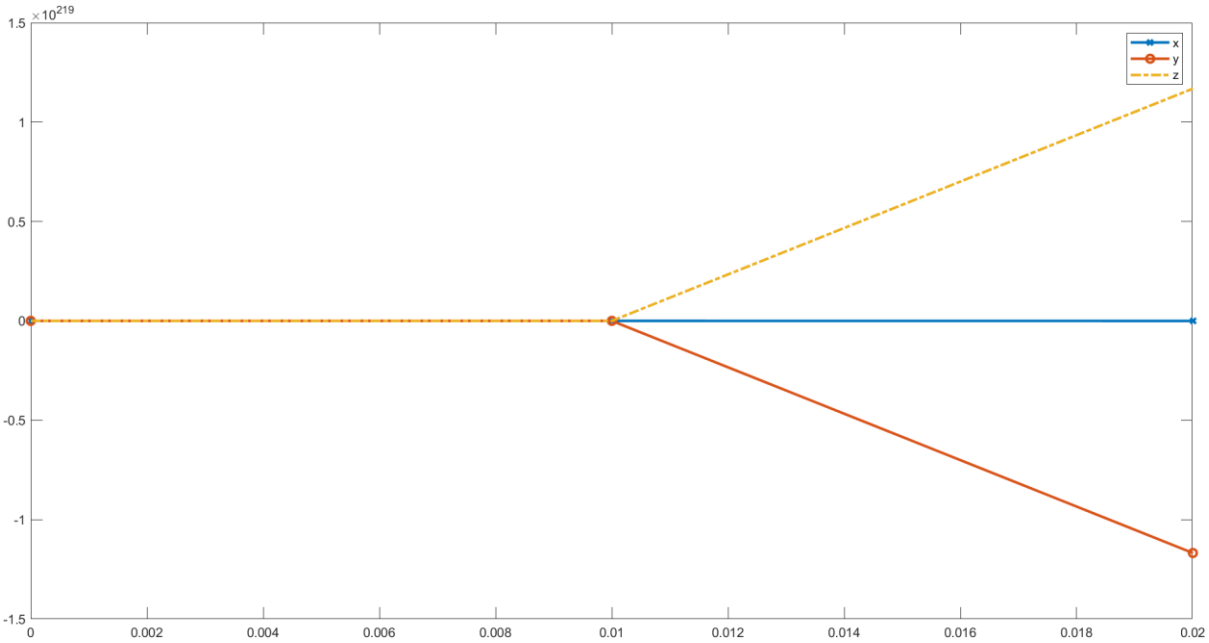
```
x = x';
y = y';
z = z';
plot(t,x,'-x','LineWidth',2);hold on;
plot(t,y,'-o','LineWidth',2);hold on;
plot(t,z,'-.','LineWidth',2);
legend('x','y','z');

function dXdt = func(t,x,y,z)
dXdt = [-0.04*x+(10^4)*y*z;
        0.04*x-(10^4)*y*z-(3*(10^7))*(y^2);
        (3*(10^7))*(y^2)];
end
```

Results



Plot generated with ode15s method



Plot generated with multivariable 4th order RK method

Conclusion

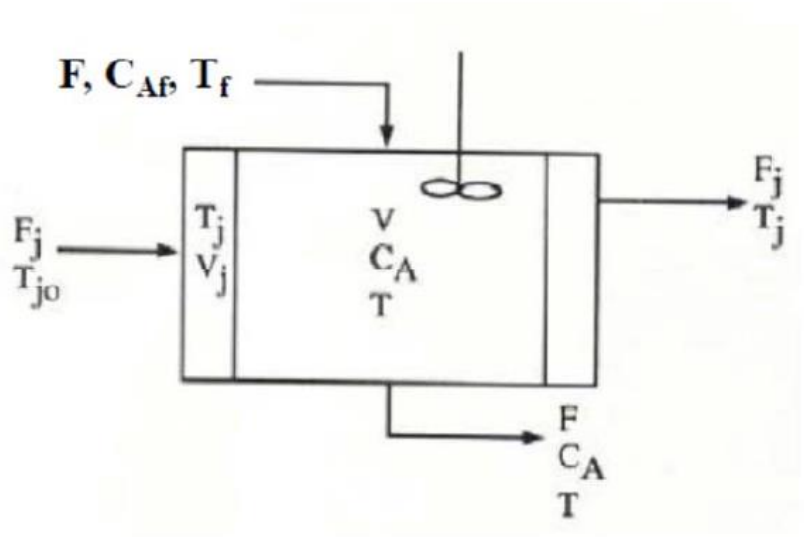
As evident from the plot obtained with the 4th order Runge-Kutta Method, the given system of differential equations is a stiff system. It means that for this method, it is highly unstable and doesn't give desired results. Usually, one solution to such problems is by lowering the step size to a very small number but here the stiffness persists even at h values as low as 0.01. The system was tested with h = 1, h = 0.1, and h =0.01 but returned stiff results every time. However, ode15s uses a multistep solver in its algorithm which can override the stiffness of a system and return consistent results. Both methods take nearly the same computational time but Runge-Kutta method will require more amount of memory because of an unusual step size which will lead to a very large solution data set.

Q.3

Problem Statement

3. Consider again the problem in Assignment – 2. The perfectly mixed CSTR where a first-order exothermic irreversible reaction takes place (r = rate of reaction).

$$A \rightarrow B, \quad r = k_0 e^{\left(\frac{-E}{RT}\right)} C_A$$



Heat generated by reaction is being removed by the jacket fluid. The reactor volume (V) is constant.

Governing Equations:

(Subscript j indicates parameters related to jacket. Symbols carry their usual significance. Refer to the figure.)

$$V\frac{dC_A}{dt} = FC_{Af} - FC_A - rV$$

$$\rho C_p V\frac{dT}{dt} = \rho C_p F\left(T_f - T\right) + \left(-\Delta H\right)Vr - UA\left(T - T_j\right)$$

$$\rho_j C_j V_j\frac{dT_j}{dt} = \rho_j C_j F_j\left(T_{j0} - T_j\right) + UA\left(T - T_j\right)$$

Model Parameter Values:

Parameter	Value	Parameter	Value
F (m^3/h)	1	C_{Af} (kgmol/m^3)	10
V (m^3)	1	UA (kcal/°C h)	150
k_0 (h^{-1})	36×10^6	T_{j0} (K)	298
($-\Delta H$) (kcal/kgmol)	6500	($\rho_j C_j$) (kcal/m^3 °C)	600
E (kcal/kgmol)	12000	F_j (m^3/h)	1.25
(ρC_p) (kcal/m^3 °C)	500	V_j (m^3)	0.25
T_f (K)	298		

Given the above parameter values, there are three steady states for this system. Perform linear stability analysis for the obtained 3 steady states. If you are not familiar with linear stability analysis, please open any process control/dynamics book.

Here are the key steps for a system with 2 state variables (C_A and reactor temperature, T). You have to extend it for 3 state variables (including jacket temperature as another state variable). Linearize the nonlinear differential equations around the steady states. Introduce deviation variables, and write the linearized ODE as follows (state space model).

$$\begin{bmatrix} \frac{dc'_A}{dt} \\ \frac{dT'}{dt} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} c'_A \\ T' \end{bmatrix} + \begin{bmatrix} 0 \\ b_2 \end{bmatrix} T'_j$$

The elements of matrix A will be: $$A_{ij} = \left.\frac{\partial f_i}{\partial x_j}\right|_{\text{steady state}}$$

Here f represents differential equation and x represent state variables. If all the eigenvalues of matrix A are negative, the system is stable. If any eigenvalue is positive, the system is unstable.

You can use MATLAB command `eig(A)` to find eigenvalues of matrix A.

Present your results using a table as follows:

Steady State (C_A, T, T_j)	Eigenvalues of Linearized System	Stable/Unstable

MATLAB Code

```
clear all;

R=1.987;
F=1;
Vj=0.25;
V=1;
k0=36000000;
H=6500;
E=12000;
rhoCp=500;
Tf=298;
Caf=10;
UA=150;
Tj0=298;
rhojCj=600;
Fj=1.25;
A=zeros([20,3]);
for i=1:20  %Finding steady states
    options=optimoptions('fsolve','Display','off');
%Supressing the output
    z=[];
    z(1)=0+rand*(10);    %Intial Guesses
    z(2)=298+rand*(100);
    z(3)=298+rand*(100);
    A(i,1:3)=fsolve(@cstrsteady,z,options); %Solving the
function
```

```
end
A=round(A,6);%Rounding the variables to 6 decimal places
Cs=A(:,1);
Ts=A(:,2);
Tjs=A(:,3);
Cs=unique(Cs,'stable');  %Finding only unique values and
stores them in the order that is found in sol.
Ts=unique(Ts,'stable');
Tjs=unique(Tjs,'stable');
A=([Cs Ts Tjs])
syms Ca T Tj
%Forming the equations
dCdt=(F/V)*(Caf-Ca)-k0*exp(-E/(R*T))*Ca;
dTdt=(rhoCp*F*(Tf-T)+H*V*k0*exp(-E/(R*T))*Ca-UA*(T-
Tj))/(rhoCp*V);
dTjdt=(Fj/Vj)*(Tj0-Tj)+(UA/(rhojCj*Vj))*(T-Tj);
Cas=A(:,1);
Ts=A(:,2);
Tjs=A(:,3);
C=zeros([3 3 3]);
for i=1:3 %Finding the value of derivative at steady
state
    C(1,1,i) = double(subs(diff(dCdt,Ca),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(1,2,i) = double(subs(diff(dCdt,T),[Ca T Tj],[Cas(i)
Ts(i) Tjs(i)]));
    C(1,3,i) = double(subs(diff(dCdt,Tj),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(2,1,i) = double(subs(diff(dTdt,Ca),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(2,2,i) = double(subs(diff(dTdt,T),[Ca T Tj],[Cas(i)
Ts(i) Tjs(i)]));
    C(2,3,i) = double(subs(diff(dTdt,Tj),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(3,1,i) = double(subs(diff(dTjdt,Ca),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(3,2,i) = double(subs(diff(dTjdt,T),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
    C(3,3,i) = double(subs(diff(dTjdt,Tj),[Ca T
Tj],[Cas(i) Ts(i) Tjs(i)]));
end
Eig=zeros([3,3]);
for i=1:3
    Eig(i,:)=eig(C(:,:,i));
end
Eig
for i=1:3  %Checking for stability of steady states
```

```
    if real(Eig(i,:))<0
        fprintf("The steady state [%f,%f,%f] is
stable\n",A(i,1),A(i,2),A(i,3));
    else
        fprintf("The steady state [%f,%f,%f] is not
stable\n",A(i,1),A(i,2),A(i,3));
    end
end

function f=cstrsteady(x)

    R=1.987;
F=1;
Vj=0.25;
V=1;
k0=36*1e6;
H=-6500;
E=12000;
Rho_Cp=500;
Tf=298;
CAf=10;
UA=150;
Tj0=298;
Rhoj_Cj=600;
Fj=1.25;
Cs=x(1);
Ts=x(2);
Tjs=x(3);
r = k0 * exp(-E/(R*Ts))*Cs;
    f(1)=F*CAf-F*Cs-r*V;
    f(2)=Rho_Cp*F*(Tf-Ts)-H*V*r-UA*(Ts-Tjs);
    f(3)=Rhoj_Cj*Fj*(Tj0-Tjs)+UA*(Ts-Tjs);
end
```

Results

Steady State (Ca, T, T_j)	Eigenvalues of Linearized System	Stable/Unstable
(1.4094, 387.3423, 312.8904)	(-1.9597+0.74i, -1.9597-0.74i, -59805)	Asymptotically Stable
(6.1650, 337.8844, 304.6474)	(0.6650, -0.911, -6.0387)	Unstable
(8.9686, 308.7270, 299.7878)	(-0.5765, -0.9355, -6.0534)	Asymptotically Stable

Conclusion

This stability test is to distinguish between the numerous critical points that exist for a system. According to our tests performed above, the 2nd steady state obtained came out to be unstable with the first eigen value being greater than the other 2 and the other 2 being < 0. This implies that such a critical point is geometrically a saddle point. Such tests can be used to classify each critical point and understand their geometrical characteristics too. The last steady state has all eigen values < 0 and therefore, gives an asymptotically stable system and so does the first steady state. The only difference being that the nature of the third steady state's critical points is that of a sink whereas, the first one is an inward spiral.