CAPE Laboratory Assignment-2

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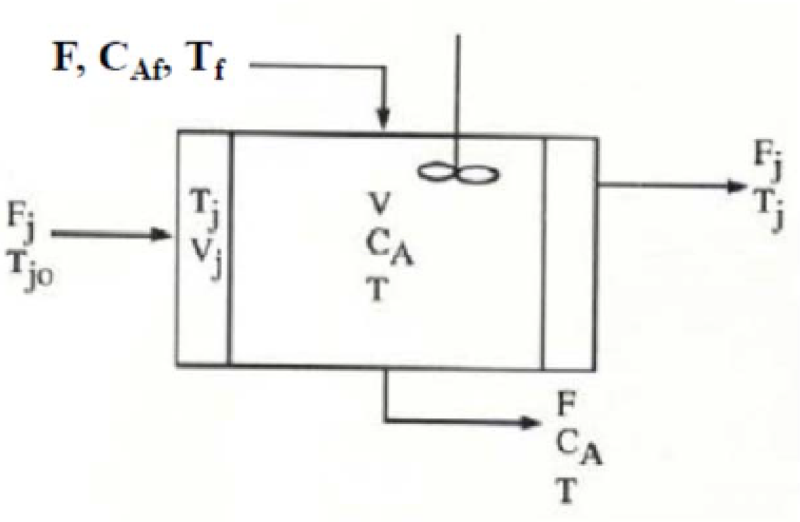
Problem Statement

1. Consider 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.

<u>Governing Equations</u>:

(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. Identify all the steady states by setting LHS of the above ODE to zero and then solving the resulting algebraic equations simultaneously for (C_A, T, T_j) by using:

1. Newton's method. Write your own code using any programming language.
2. MATLAB function `fsolve`.
3. Compare your results (all 3 steady states) obtained by two methods in a Table.

Use of MATLAB function `fsolve`:

First write the function to describe the 3 algebraic equations and save it as `cstrsteady.m`

```
function F = cstrsteady(x)

F(1) = ....
F(2) = ....
F(3) = ....
```

Next execute the following command:

```
X0 = .... % Initial guess
xout = fsolve(@cstrsteady, X0)
```

`xout` contains the solution (steady state). Note it is a vector with 3 elements.

MATLAB Code

Multivariable Newton Raphson

```
clear all;

global k0 Ea R;
k0 = 36*10^6;
Ea = 12000;
R = 2;
Xi = [5; 300; 400]; %Initial Guess
for i= 1:50
 [f, jacobian] = cstr(Xi);
 Xsol = Xi - inv(jacobian)*f; %Multivariable Newton
Raphson Method statement

 if(abs(Xi-Xsol)<=10^-4) %Tolerance Check
 break;
 end
 Xi=Xsol;
end

function [Func,j_val] = cstr(X) %Equations
global k0 Ea R;
F = 1;
Rho_Cp= 500; % Model Parameter Values
UA=150;
Tj0=298;
Fj=1.25;
Tf = 298;
Rhoj_Cpj=600;
V=1;
CAf=10;
deltaH = 6500;
CA = X(1);
```

```
T = X(2);
Tj = X(3);
r = k0 * exp(-Ea/(R*T))*CA ;
Func(1, 1) = F*CAf - F*CA - r*V ;
Func(2, 1) = Rho_Cp*F*(Tf-T) + deltaH*V*r - UA*(T - Tj);
Func(3, 1) = Rhoj_Cpj*Fj*(Tj0 - Tj) + UA*(T - Tj);

syms x y z ; %Jacobian calculate
J = jacobian([10- x- k0 * exp(-Ea/(R*y))*x ; 500*(298-y)
+ 6500*(k0 * exp(-Ea/(R*y))*x) - 150*(y - z);
600*1.25*(298 - z) + 150*(y - z) ], [x y z]);
j_val = double(subs(J, [x y z], [X(1), X(2), X(3)]));
end
```

Using *fsolve* function

```
clear all;

global k0 Ea R;

k0 = 36*10^6;
Ea = 12*10^3;
R = 2;
Xi = [5; 350; 500]; %Initial Guess
xout = fsolve(@cstrsteady,Xi); % fsolve statement

function [Func] = cstrsteady(X) %Equations definition
global k0 Ea R;

F = 1;
Rho_Cp= 500; % Model Parameter Values
UA=150;
Tj0=298;
Fj=1.25;
Tf = 298;
Rhoj_Cpj=600;
V=1;
CAf=10;
deltaH = 6500;
CA = X(1);
T = X(2);
Tj = X(3);

r = k0 * exp(-Ea/(R*T))*CA ;
Func(1, 1) = F*CAf - F*CA - r*V ;
Func(2, 1) = Rho_Cp*F*(Tf-T) + deltaH*V*r - UA*(T - Tj);
Func(3, 1) = Rhoj_Cpj*Fj*(Tj0 - Tj) + UA*(T - Tj);
```

```
end
```

Results

Method	Multivariable Newton Raphson			*fsolve* function		
Variables	C_A (kgmol/m^3)	T (K)	T_j (K)	C_A (kgmol/m^3)	T (K)	T_j (K)
Steady State 1	8.4934	313.6684	300.6114	8.4934	313.6684	300.6114
Steady State 2	7.2185	326.9277	302.8213	7.2185	326.9277	302.8213
Steady State 3	1.1944	389.5785	313.2631	1.1944	389.5785	313.2631

Conclusion

For same initial guesses, *fsolve* function is seen to take less computational time as compared to the multivariable Newton-Raphson method when compared on the MATLAB profiler. However, accuracy wise both methods are observed to give same results. Care needs to be taken while defining the initial guesses because sometimes they can lead the method to diverge or even converge after a very large number of iterations, and both situations are unfavourable for us. It is to be noted that the multivariable Newton Raphson method will work only if our functions are continuous and differentiable everywhere. Since all the equations are related to one another due to presence of multiple variables, obtaining 3 steady states seems to be logical since, the system can attain steady state in multiple ways too.