In [1]:
```
import numpy as np
from scipy.integrate import odeint
from scipy.optimize import fsolve, curve_fit
from matplotlib import pyplot as plt
from scipy.integrate import solve_ivp
```

CPN Project Task A

Group 7

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Task 2 – System Identification:

System Variable	Assigned Variable
(1) Manipulated variable	Stem position of the valve
(2) Control variable	Production rate of ammonia
(3) Disturbance variable	Feed Composition
(4) Final control element	Valve

Reasons for assigning System variable (1)-(4):

1. It can be easily controlled by adjusting the position of the valve.
2. We are told to produce high volumes of ammonia no matter what.
3. The boss has told us the feed composition can vary and this is a disturbance.
4. By adjusting the valve, the flowrate to the reactor (manipulated variable) changes.

Task 3 – System Equations and Assumptions:

Assumptions

The reactor tank is well mixed

Physical properties stays constant

The system is initially at steady state

K is only Temperature dependant

Flow into the reactor is dependant on the valve opening

Conservative Equations

$$\frac{dy(t)}{dt} = \frac{K_p Ps(t)}{\tau^2} - \frac{2\zeta y(t)}{\tau} - \frac{x(t)}{\tau^2} \qquad \ldots(1)$$
$$\frac{dx(t)}{dt} = y(t) \qquad \ldots(2)$$
$$\frac{dC_{NH_3}}{dt} = \frac{FC_{NH3,in}}{V} - \frac{FC_{NH3}}{V} + 2kC_{N_2}C_{H_2}^3 \qquad \ldots(3)$$
$$\frac{dC_{H_2}}{dt} = \frac{FC_{H2,in}}{V} - \frac{FC_{H2}}{V} - 3kC_{N_2}C_{H_2}^3 \qquad \ldots(4)$$
$$\frac{dC_{N_2}}{dt} = \frac{FC_{N2,in}}{V} - \frac{FC_{N2}}{V} - kC_{N_2}C_{H_2}^3 \qquad \ldots(5)$$

Constitutive equations

$$F = C_{cv} f(x(t)) \sqrt{\frac{\Delta P_{CV}}{SG}} \qquad \ldots(6)$$
$$f(x(t)) = \sqrt{x(t)} \qquad \ldots(7)$$
$$k = k_0 e^{-\frac{Ea}{RT}} \qquad \ldots(8)$$

DOF

Independant equations include: Equations 1, 2, 3, 6, 7, 8 = 6 Equations in total

Unknowns include: y(t), k, F, Ps(t), f(x(t)), CNH3 = 6 Unknowns in total

DOF = NV - NE = 6 - 6 = 0

System is exactly specified

Task 4 – Steady State Calculations Using Python:

In [2]:
```python
#-----------------------------------Calculating volumetric flow-------------
MM = np.array([14.0067*2, 1.00784*2])
molar_fractions = np.array([0.25, 0.75])
MM_mix = MM[0]*molar_fractions[0] + MM[1]*molar_fractions[1]   #g/mol
molar_flow = 1304.85    #mol/s from Task 1
mass_flow = molar_flow*MM_mix / 1000   #kg/s
density_mix = 8.81609     #kg/m^3 from Task 1
volumetric_flow = mass_flow/density_mix #m^3/s

#------------------------------------------Known variables-----------------
V = 1
k0 = 0.0001
Ea = 60000
R = 8.314
T = 1140   #from Task 1
k = k0*np.exp(-Ea/(R*T))
F = volumetric_flow
CN2_in = molar_flow * molar_fractions[0] / F
CH2_in = molar_flow * molar_fractions[1] / F
CNH3_in = 0

#------------------------------------------Using fsolve--------------------
def solve(y):
    CN2, CH2, CNH3 = y
    eqn1 = F*CN2_in/V - F*CN2/V - k*CN2*CH2**3
    eqn2 = F*CH2_in/V - F*CH2/V - 3*k*CN2*CH2**3
    eqn3 = F*CNH3_in/V - F*CNH3/V + 2*k*CN2*CH2**3
    return eqn1, eqn2, eqn3
guess = [CN2_in/2, CH2_in/2, CN2_in*2]   #Guess values are chosen which shou
CN2_ss, CH2_ss, CNH3_ss = fsolve(solve,guess)
print("SS conc N2 = {} mol/m^3, SS conc H2 = {} mol/m^3, SS conc NH3 = {} mo
print('SS molar flow N2 = {} mol/s, SS molar flow H2 = {} mol/s, SS molar fl
```

```
SS conc N2 = 82.45 mol/m^3, SS conc H2 = 247.36 mol/m^3, SS conc NH3 = 352.
76 mol/m^3
SS molar flow N2 = 103.92 mol/s, SS molar flow H2 = 311.75 mol/s, SS molar
flow NH3 = 444.59 mol/s
```

The results of the above calculations are given in the table below

Variable	Value	Units
Concentration of N2	82.45	mol/m³
Concentration of H2	247.36	mol/m³
Concentration of NH3	352.76	mol/m³
Flow rate	1.260	m³/s

Task 5 – Steady State Simulation Using DWSIM:

Variable	Python	DWSIM value	Units
Molar flow of N2	103.92	103.90	mole/s
Molar flow of H2	311.75	311.70	mole/s
Molar flow of NH3	444.59	444.63	mole/s
Flow rate	1.26	0.83	m3/s

Conversion used in DWSIM is 68.15%

Task 6 – Transient System Response:

In [8]:
```
#-----------------------------------------Known variables------------------
tau = 10   #s
Kp = 1/12
zeta = 3
P_initial = 9
del_P = 2
#---------------------------------------Initial calculations---------------
x_initial = Kp*P_initial
SG = density_mix / 997
Cv = volumetric_flow / np.sqrt(x_initial) / np.sqrt(2/SG)
#-----------------------------------------Chosen variables-----------------
M = 4   #Chosen step change in pressure
t_end = 400  #Time to integrate to
steps = 10000    #Steps for integration
t_step_change = 50    #Time at which the pressure undergoes a step change

#---------------------------Solver function---------------------------------
def euler_solver(t_end, steps, t_step_change, M):
#-----------------------------------------Initialize values----------------
```

```
    times = np.linspace(0, t_end, steps)
    dt = times[1] - times[0]
    Ps = np.zeros(len(times))    #These arrays will be updated in the for lo
    x = np.zeros(len(times))    #These arrays will be updated in the for loo
    y = np.zeros(len(times))    #These arrays will be updated in the for loo
    Fs = np.zeros(len(times))    #These arrays will be updated in the for lo
    CN2 = np.zeros(len(times))    #These arrays will be updated in the for l
    CH2 = np.zeros(len(times))    #These arrays will be updated in the for l
    CNH3 = np.zeros(len(times))    #These arrays will be updated in the for

    Ps[0] = P_initial     #The initial conditions can be changed outside the
    x[0] = x_initial     #The initial conditions can be changed outside the
    y[0] = 0     #The initial conditions can be changed outside the functior
    Fs[0] = volumetric_flow     #The initial conditions can be changed outsi
    CN2[0] = CN2_ss     #The initial conditions can be changed outside the i
    CH2[0] = CH2_ss     #The initial conditions can be changed outside the i
    CNH3[0] = CNH3_ss     #The initial conditions can be changed outside the
#---------------------------------------------For loop----------------------
    for i in range(0, len(times)-1):
#----------------------------------Get pressures with step change-----------
        if times[i] <= t_step_change:
            Ps[i+1] = P_initial
        else:
            Ps[i+1] = P_initial + M
#-----------------------------------------Solve for x values----------------
        dxdt = y[i]
        dydt = -2*zeta/tau*dxdt - x[i]/tau**2 + Kp*Ps[i]/tau**2
        x[i+1] = x[i] + dxdt*dt
        y[i+1] = y[i] + dydt*dt
#----------------------------------------Calculating flowrate---------------
        Fs[i+1] = Cv * x[i+1]**0.5 * np.sqrt(2/SG)
#--------------------------------------Solve for concentrations-------------
        dcn2dt = Fs[i]*(CN2_in - CN2[i]) - k*CN2[i]*CH2[i]**3
        dch2dt = Fs[i]*(CH2_in - CH2[i]) - 3*k*CN2[i]*CH2[i]**3
        dcnh3dt = Fs[i]*(CNH3_in - CNH3[i]) + 2*k*CN2[i]*CH2[i]**3
        CN2[i+1] = CN2[i] + dcn2dt*dt
        CH2[i+1] = CH2[i] + dch2dt*dt
        CNH3[i+1] = CNH3[i] + dcnh3dt*dt

    return times, Ps, x, Fs, CN2, CH2, CNH3

times, Ps, x, Fs, CN2, CH2, CNH3 = euler_solver(t_end, steps, t_step_change,
```

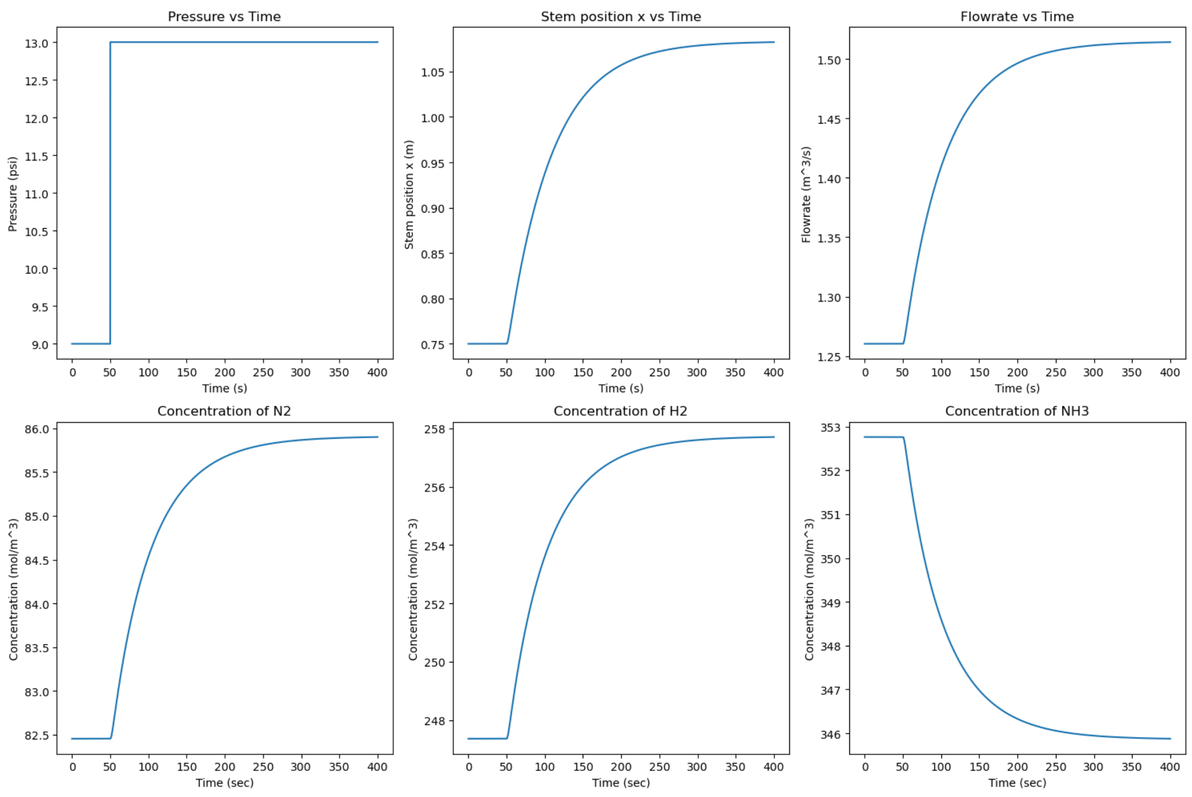
In [9]:

```
#----------------------------------------Plotting the results---------------
fig, axs = plt.subplots(2, 3, figsize=(15, 10))

axs[0, 0].plot(times, Ps)
axs[0, 0].set_title("Pressure vs Time")
axs[0, 0].set_xlabel("Time (s)")
axs[0, 0].set_ylabel("Pressure (psi)")
axs[0, 1].plot(times, x)
axs[0, 1].set_title("Stem position x vs Time")
axs[0, 1].set_xlabel("Time (s)")
axs[0, 1].set_ylabel("Stem position x (m)")
axs[0, 2].plot(times, Fs)
axs[0, 2].set_title("Flowrate vs Time")
axs[0, 2].set_xlabel("Time (s)")
axs[0, 2].set_ylabel("Flowrate (m^3/s)")
axs[1, 0].plot(times, CN2)
axs[1, 0].set_title("Concentration of N2")
axs[1, 0].set_xlabel("Time (sec)")
axs[1, 0].set_ylabel("Concentration (mol/m^3)")
axs[1, 1].plot(times, CH2)
axs[1, 1].set_title("Concentration of H2")
```

```
axs[1, 1].set_xlabel("Time (sec)")
axs[1, 1].set_ylabel("Concentration (mol/m^3)")
axs[1, 2].plot(times, CNH3)
axs[1, 2].set_title("Concentration of NH3")
axs[1, 2].set_xlabel("Time (sec)")
axs[1, 2].set_ylabel("Concentration (mol/m^3)")

plt.tight_layout()
plt.show()
```



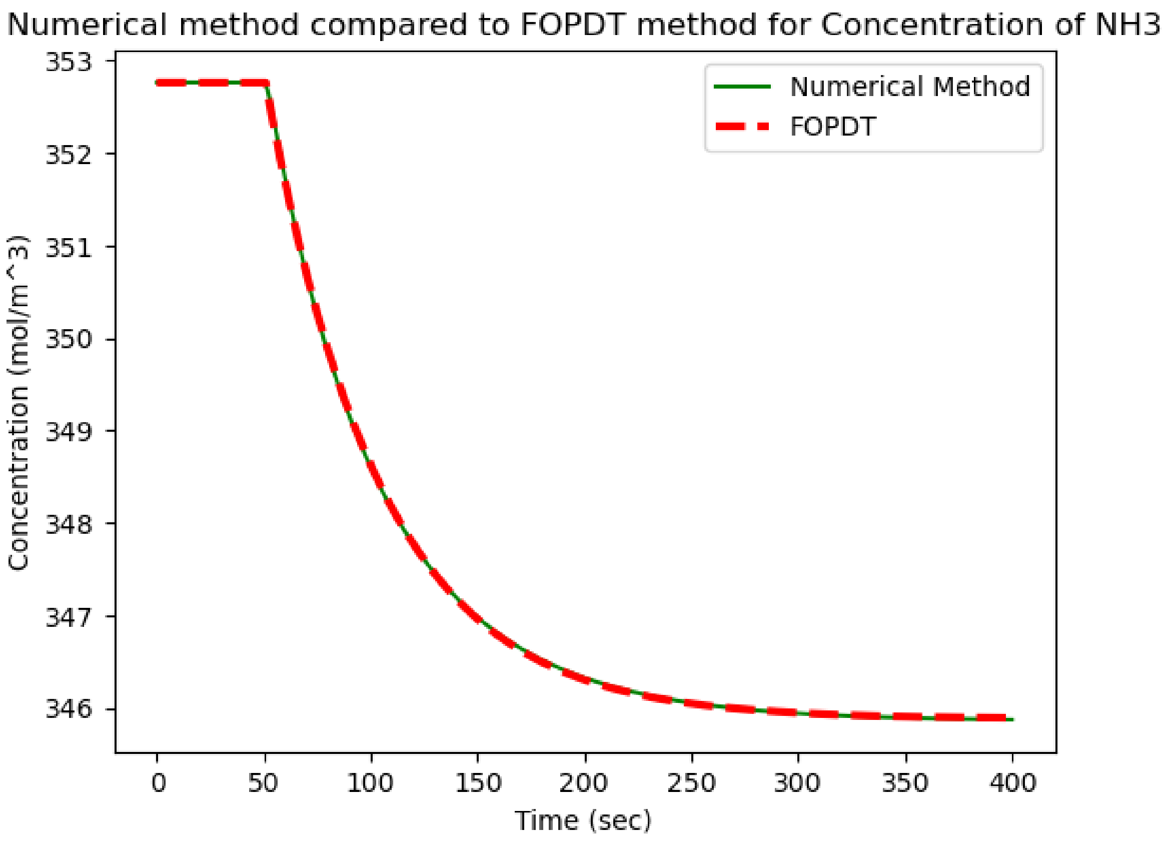
Task 7 – FOPDT Fitting and Determination of Kp, Tau and Theta:

In [10]:
```
#------------------------------------------FOPDT function--------------------
def FOPDT(t, Kp, tau, theta):
    C_vals = []
    for i in t:
        if i<=theta:
            C_vals.append(Cs)
        if i>theta:
            C = Kp*M*(1-np.exp(-(i-theta)/tau)) + Cs
            C_vals.append(C)
    return np.array(C_vals)
#------------------------------------------Guess values--------------------
Cs = CNH3[0]
Kp_guess = (CNH3[-1] - Cs)/M
tau_guess = 80     #Calculated by finding the time at which the concentratio
theta_guess = 50
#------------------------------------Solving for KP, tau and theta-----------
params,_ = curve_fit(FOPDT,times,CNH3,p0=[Kp_guess, tau_guess, theta_guess])
Kp, tau, theta_total = params
theta = theta_total - t_step_change     #The overall deadtime needs to be su
FOPDT_flows = FOPDT(times, Kp, tau, theta_total)    #Now calculate the flows
                                                    #Note we use theta_total
```

The values of Kp, tau and theta are given in the table below

Variable	Calculated value	Units
Kp	-1.866	
Tau	55.634	s
Theta	1.304	s

In [11]:
```
plt.figure()
plt.title("Numerical method compared to FOPDT method for Concentration of NH
plt.xlabel("Time (sec)")
plt.ylabel("Concentration (mol/m^3)")
plt.plot(times,CNH3,'g',label='Numerical Method')
plt.plot(times,FOPDT_flows,'r--',label='FOPDT',linewidth=3)
plt.legend(loc='best')
plt.show()
```


Numerical method compared to FOPDT method for Concentration of NH3
Numerical Method
FOPDT
Concentration (mol/m^3)
Time (sec)