HOMEWORK 2

PROBLEM 1

Homework Set 2

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a) Assuming constant density

$$\frac{dV_{sys}}{dt} = \nu_{in} - \nu_{out} + \nu_{gen}$$

During filling stage, $\nu_{in} = \nu_0$, $\nu_{out} = \nu_{gen} = 0$ $\{t < t_1\}$

$$\frac{dV}{dt} = \nu_0 \quad \text{— (1)}$$

Taking material balance of B

$$\frac{dN_B}{dt} = n_{B_{in}} - n_{B_{out}} + n_{B_{gen}}$$

$n_{B_{in}} = C_{B0}\nu_{in}$, $n_{B_{gen}} = -r_B V = -kN_B$, $n_{B_{out}} = 0$

$$\frac{dN_B}{dt} = C_{B0}\nu_0 - kN_B \quad \text{— (2)}$$

$$\frac{dN_R}{dt} = n_{R_{in}} - n_{R_{out}} + n_{R_{gen}}$$

$n_{R_{in}} = 0$, $n_{R_{out}} = 0$, $n_{R_{gen}} = r_R V = kN_B$

$$\frac{dN_R}{dt} = kN_B \quad \text{— (3)}$$

$$t_1 = \frac{V_f - V_0}{\nu_0}$$

After filling $\{t \geq t_1\}$

$$\frac{dV_{sys}}{dt} = \nu_{in} - \nu_{out} + \nu_{gen}$$

$\nu_{in} = 0$ {stops filling up}

$\nu_{out} = 0$

$\nu_{gen} = 0$

$$\frac{dV}{dt} = 0 \quad \text{— (4)}$$

$$\frac{dN_B}{dt} = n_{B_{in}} - n_{B_{out}} + n_{gen}$$

$n_{B_{in}} = 0$, $n_{B_{gen}} = -r_B V = -kC_B V = -kN_B$, $n_{B_{out}} = 0$

$$\frac{dN_B}{dt} = -kN_B \quad \text{— (5)}$$

$$\frac{dN_R}{dt} = r_{in} - r_{out} + r_{gen}$$

$r_{in} = 0$, $r_{out} = 0$, $r_{gen} = k C_{B/V} = k N_B$

$$\frac{dN_R}{dt} = k N_B \quad \text{—— (6)}$$

b) From eqn (2)

$$\frac{dN_B}{dt} = C_{B0} V_0 - k N_B \quad , N_{B0} = N_{R0} = 0$$

Seperating variables,

$$\int_{N_{B0}}^{N_B(t)} \frac{dN_B}{C_{B0} V_0 - k N_B} = \int_0^t dt$$

$$-\frac{1}{k} \ln \frac{(C_{B0} V_0 - k N_B)}{C_{B0} V_0} \Bigg|_{N_{B0}=0}^{N_B(t)} = t$$

$$\ln \frac{(C_{B0} V_0 - k N_B(t))}{(C_{B0} V_0)} = -kt$$

$$C_{B0} V_0 - k N_B(t) = C_{B0} V_0 \exp(-kt)$$

$$\boxed{N_B(t) = \frac{C_{B0} V_0}{k} (1 - \exp(-kt))} \quad \text{—— II}$$

$$\frac{dN_R}{dt} = k N_B = C_{B0} V_0 (1 - \exp(-kt))$$

$$N_R(t) = \int_0^t C_{B0} V_0 (1 - \exp(-kt)) \, dt$$

$$N_R(t) = C_{B0} V_0 \left(t + \frac{\exp(-kt)}{k}\right) \Bigg|_0^t$$

$$\boxed{N_R(t) = C_{B0} V_0 \left(t + \frac{1}{k} (\exp(-kt) - 1)\right)} \quad \text{—— III}$$

From eqn (5)

$$\frac{dN_B}{dt} = -k N_B$$

From eqn (2), at s-s $dN_B/dt = 0$

$$N_{B_{s\text{-}s}} = N_{B_1} = \frac{C_{B0} V_0}{k}$$

Seperating variables, $\displaystyle\int_{N_{B_1}}^{N_B(t)} \frac{dN_B}{N_B} = \int_{t_1}^{t} -k \, dt$

$$\ln \frac{N_B(t)}{N_{B_1}} = -k(t - t_1)$$

$$\boxed{N_B(t) = N_{B_1} \exp(-k(t-t_1))} \quad \text{— (V)}$$

From eqn (6)

$$\frac{dN_R}{dt} = k N_B = k N_{B_1} \exp(-k(t-t_1))$$

$$N_R(t) = \int_{t_1}^{t} k N_{B_1} \exp(-k(t-t_1))\, dt$$

$$N_R(t) = \int_{t_1}^{t} C_{B_0} v_0 \exp(-k(t-t_1))\, dt$$

$$\boxed{N_R = v_0 C_{B_0} \left[t_1 - 1/k(1-\exp(-kt_1))\exp(-k(t-t_1)) \right]} \quad \text{— (VI)}$$

Matlab Code

```
clc clf clear
global k Cbo Vo vo V1 t1 Nb1
k =0.1;%min^1
Cbo = 1; %M
vo = 25; %L/min
Vo = 5;  %L
V1 = 255; %L
Yo = [Vo 0 0];
t1 = (V1 - Vo)./vo;
Nb1 = ((vo*Cbo)./k)*(1-exp(-k*t1));
t0 = 0;
tf = 25.0;
tspan = [t0 tf];

[t, Y] = ode45('No1deriv', tspan, Yo);     % for "ode45" solver
t2 = linspace(1,25,25);
for i = 1:25
      Xa(i,:) = No1ana(i);
end
plot (t, Y(:,1), '-',t, Y(:,2), '-',t, Y(:,3), '-',
t2,Xa(:,1),'o',t2,Xa(:,2),'o',t2, Xa(:,3),'o'),. . .
title ('Concentration vs Time'), ...
legend ('V', 'N_B', 'N_R', 'Va', 'N_Ba', 'N_Ra'),
xlabel ('t, min'),
ylabel ('V (L), N_B (mol), N_R (mol), Va (L), N_Ba
(mol), N_Ra (mol)');

function dY = No1deriv(t,Y)
global k Cbo Vo vo V1 t1 Nb1

if (t < t1)
    dV = vo;
    dNb = vo * Cbo - k * Y(2);
    dNr = k * Y(2);
end
```

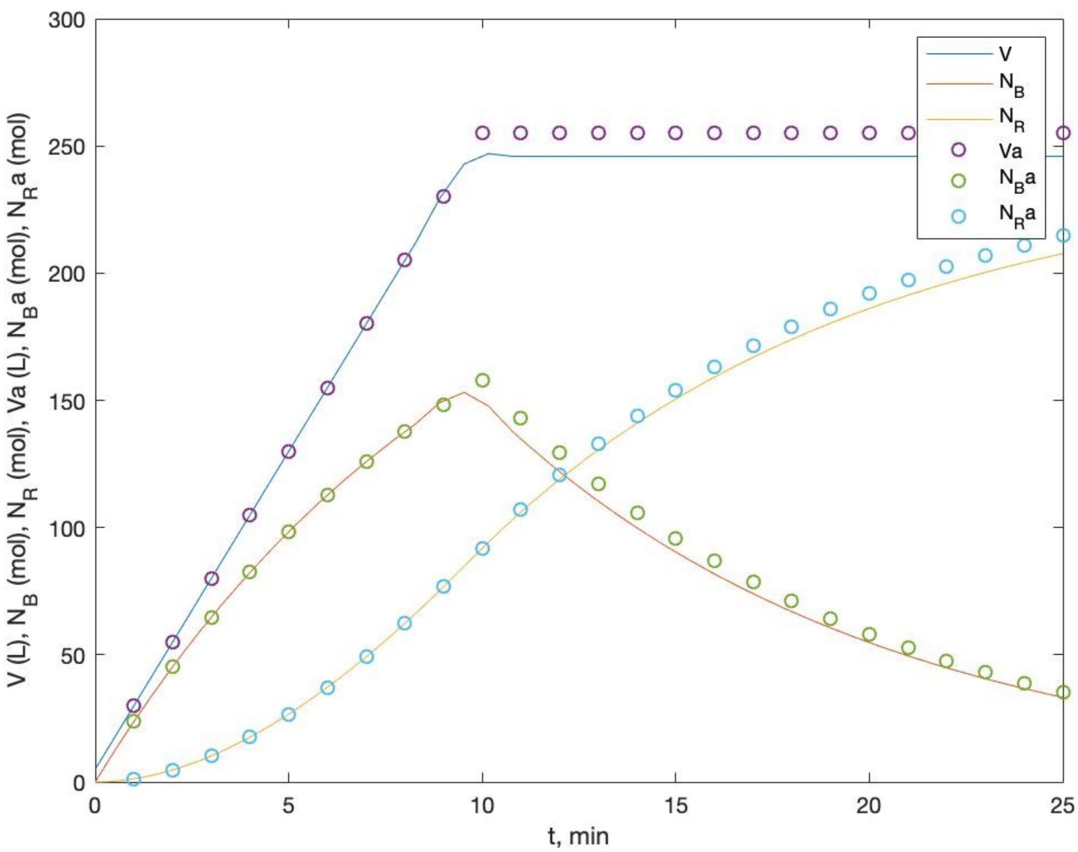
```
if (t >= t1)
    dV = 0;
    dNb = - k * Y(2);
    dNr = k * Y(2);
end
dY = [dV; dNb; dNr];

function X = No1ana(t)
global k Cbo Vo vo V1 t1 Nb1

if (t < t1)
    X(1) = Vo + vo*t;
    X(2) = ((vo * Cbo)./k)*(1-exp(-k*t));
    X(3) = (vo * Cbo)*(t + 1/k.*(exp(-k*t)-1));
end

if (t >= t1)
    X(1) = V1;
    X(2) = Nb1*exp(-k*(t-t1));
    X(3) = (vo * Cbo)*(t1 - 1/k.*(1-exp(-k*t1))*exp(-k*(t-t1)));
end

X = [X(1) X(2) X(3)]
```



PROBLEM 2

$$CO_2 \underset{}{\overset{K_1}{\rightleftharpoons}} CO + 0.5O_2$$

$$0.5O_2 + 0.5N_2 \underset{}{\overset{K_2}{\rightleftharpoons}} NO$$

$T = 3000K$ $\quad P = 10\,atm$

$K_1 = 0.3272$ $\quad K_2 = 0.1222$

Feed = 4 mol/min

$CO_2, O_2, N_2 \Rightarrow 2:1:1 \Rightarrow$ 2mol/min, 1mol/min, 1mol/min

Atomic Species $\Rightarrow$ C, O, N

Carbon Balance:

$$\frac{1\,g\text{-atom}}{mol} F_{CO_2} + \frac{1\,g\text{-atom}}{mol} F_{CO} - \frac{1\,g\text{-atom}}{mol} \frac{2\,mol}{min} = 0$$

$$\boxed{F_{CO_2} + F_{CO} - 2 = 0}$$

Oxygen Balance:

$$\frac{2\,g\text{-atom}}{mol} F_{CO_2} + \frac{1\,g\text{-atom}}{mol} F_{CO} + \frac{2\,g\text{-atom}}{mol} F_{O_2} + \frac{1\,g\text{-atom}}{mol} F_{NO}$$

$$- \frac{2\,g\text{-atom}}{mol} \frac{2\,mol}{min} - \frac{2\,g\text{-atom}}{mol} \frac{1\,mol}{min} = 0$$

$$\boxed{2F_{CO_2} + F_{CO} + 2F_{O_2} + F_{NO} - 6 = 0}$$

Nitrogen Balance:

$$\frac{2\,g\text{-atom}}{mol} F_{N_2} + \frac{1\,g\text{-atom}}{mol} F_{NO} - \frac{2\,g\text{-atom}}{mol} \frac{1\,mol}{min} = 0$$

$$\boxed{2F_{N_2} + F_{NO} - 2 = 0}$$

$$K_1 = \frac{a_{CO} \cdot a_{O_2}^{0.5}}{a_{CO_2}} = \frac{\left(\frac{y_{CO} P_{tot}}{1atm}\right)\left(\frac{y_{O_2} P_{tot}}{1atm}\right)^{0.5}}{\left(\frac{y_{CO_2} P_{tot}}{1atm}\right)}$$

$$K_1 = \frac{\left(F_{CO}/F_{tot}\right)\left(F_{O_2}/F_{tot} \cdot \frac{P_{tot}}{1atm}\right)^{0.5}}{F_{CO_2}/F_{tot}} = \boxed{\frac{F_{CO} \times F_{O_2}^{0.5}}{F_{CO_2} \times F_{tot}^{0.5}} \left[\frac{P_{tot}}{1atm}\right]^{0.5}}$$

$$K_2 = \frac{a_{NO}}{a_{O_2}^{0.5} \cdot a_{N_2}^{0.5}} = \frac{\left(\frac{y_{NO} P_{tot}}{1atm}\right)}{\left(\frac{y_{O_2} P_{tot}}{1atm} \cdot \frac{y_{N_2} P_{tot}}{1atm}\right)^{0.5}} = \frac{F_{NO}/F_{tot}}{\left(F_{O_2}/F_{tot} \cdot F_{N_2}/F_{tot}\right)^{0.5}}$$

$$\boxed{K_2 = \frac{F_{NO}}{\left(F_{O_2} \cdot F_{N_2}\right)^{0.5}}}$$

Equilibrium composition of effluents: $F_{CO_2} = 1.5388$ mol/min $\quad F_{CO} = 0.4612$ mol/min

$F_{O_2} = 0.4125$ mol/min $\quad F_{N_2} = 0.9513$ mol/min $\quad F_{NO} = 0.0774$ mol/min

Matlab Code

```
% F(1) = FCO2, F(2) = FCO, F(3) = FO2, F(4) = FN2, F(5) = FNO, function
G = No2main(F)
FTot = (F(1)) + (F(2)) + (F(3)) + (F(4)) + (F(5)); % mol/h
PTot = 10.0; % atm
K1 = 0.3272; % Rxn 1 eqm constant
K2 = 0.1222; % Rxn 2 eqm constant
G = [F(1) + F(2) - 2; % C balance
     3*F(1) + F(2) + 2*F(3) + F(5) - 6; % O balance
     2*F(4) + F(5) + - 2; % N balance
     F(2)*(F(3)^0.5)*(PTot^0.5)/(F(1)*(FTot^0.5)) - K1; % Rxn 1 equilibrium
     ((F(5))/(F(1)*F(3))^0.5) - K2]; % Rxn 2 equilibrium
End
function No2fzero F0 =
[1 1 1 1 1]; % mol/h
options=optimset('Display','iter'); % Option to display output
[F,fval,exitflag_imp]= fsolve(@No2main, F0, options) end
  Output
gives:

F =  1.5388    0.4612    0.4125    0.9513    0.0974

fval =
     1.0e-
10 *

    0.0006    -
0.0001
    0.0000
0.1531
    0.0157

exitflag_imp =

     1
```

Equilibrium Compositions =>

FCO2 = 1.5388 mol/min
FCO = 0.4612 mol/min
FO2 = 0.4125 mol/min   FN2
= 0.9513 mol/min
FNO = 0.0974 mol/min