# Taller 4.

```
clear
%Datos suministrados por el ejercicio
FC_out = 700 ; % kg/dia
MWC = 90 ; %kg/kmol
yA0 = 0.75 ;
T0 = 350 ; %°C
T0 = T0 + 273.15 ; %K
P0 = 4 ;%bar
P0 = P0*100000 ; %Pa
xA = 0.85 ;

%Cálculos preliminares
R = 8.3145 ; % Pa*m3/(mol*K)
FA0 = FC_out/MWC*2/0.5/xA ;% kmol/dia
FA0 = FA0*(1/24)*(1/60)*(1/60)*(1000)  % mol/s
```

```
FA0 = 0.4236
```

```
FT0 = FA0/yA0 % mol/s
```

```
FT0 = 0.5648
```

```
Q0 = R*FT0*T0/P0 % (Pa*m3)/(mol*K)*(mol/s)*(K)/(Pa) = m3/s
```

```
Q0 = 0.0073
```

$$2A \longrightarrow B + 0.5C$$

La rápidez de reacción es

$$r_A = -k(T)C_A = \frac{k(T)F_A}{Q}$$

Como es una reacción en fase gaseosa, el caudal no es constante.

**SUPOSICIONES:**

- Se comportan como gases ideales
- Es una operación isotérmica (T=T0)
- No se contemplan caídas de presión(P=P0)

Luego

$$Q_0 = \frac{F_{T0}RT_0}{P_0}$$

$$Q = \frac{F_T RT}{P}$$

Por tanto

$$\frac{Q}{Q_0} = (\frac{F_T}{F_{T0}})(\frac{T}{T_0})(\frac{P_0}{P}) = \frac{F_T}{F_{T0}}$$

Por el balance de materia:

$$F_{A,out} = F_{A,in}(1 - x_A)$$

$$F_{B,out} = \frac{F_{A,in}}{2} x_A$$

$$F_{C,out} = \frac{F_{A,in}}{4} x_A$$

$$F_{inertes,out} = F_{inertes,in}$$

$$\longrightarrow F_T = F_{A,in} + F_{inertes} - 0.25 F_{A,in} x_A = F_{T0} - 0.25 F_{A,in} x_A$$

Por tanto,

$$\longrightarrow \frac{F_T}{F_{T0}} = 1 - 0.25 \frac{F_{A,in}}{F_{T0}} x_A = 1 - 0.25 y_{A,0} x_A$$

Siendo posible escribir

$$Q = Q_0(1 - 0.25 y_{A,0} x_A)$$

y, por tanto

$$r_A = -k(T) \frac{F_{A,0}(1 - x_A)}{Q_0(1 - 0.25 y_{A,0} x_A)}$$

```
%Cinética
k = @(T) exp(33.33-24250./T) ; %1/s
rA = @(T,xA) -k(T)*FA0*(1-xA)./(Q0*(1-0.25*yA0*xA)) ; %mol/s/m3
```

## A. Dos reactores CSTR en paralelo $V_1 = V_2$

El balance de materia en el reactor es

$$F_{A,0} - F_{A,1} + r_{A,(T,x_{A,1})} V_1 = F_{A,0} x_{A,1} + r_{A,(T,x_{A,1})} V_1 = 0$$

$$F_{A,1} - F_{A,2} + r_{A,(T,x_{A,2})} V_2 = F_{A,0}(1 - x_{A,1}) - F_{A,0}(1 - x_{A,2}) + r_{A,(T,x_{A,2})} V_2 = F_{A,0}(x_{A,1} - x_{A,1}) + r_{A,(T,x_{A,2})} V_2 = 0$$

Como $V_1 = V_2$, entonces

$$V = \frac{-F_{A,0} x_{A,1}}{r_{A,(T,x_{A,1})}} = \frac{-F_{A,0}(x_{A,2} - x_{A,1})}{r_{A,(T,x_{A,2})}}$$

Donde $x_{A,2} = 0.85$, la única variable es $x_{A,1}$, luego

```
xA1a = fsolve(@(xA1) FA0*(-xA1/(rA(T0,xA1))+(xA-xA1)/(rA(T0,xA))),0.5)
```

```
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.

<stopping criteria details>
xA1a = 0.6064
```

```
Va = -FA0*xA1a/rA(T0,xA1a) %m3
```

```
Va = 2.6616
```

```
Vtotala = 2*Va
```

```
Vtotala = 5.3232
```

## B. Dos reactores CSTR en paralelo (Flujo dividido en partes iguales). $V_1 = 0.75V_2$

Realizamos los balances de materia

$$F_{A,01} - F_{A,11} + r_{A,(T,x_{A,1})}V_1 = F_{A,01}x_{A,1} + r_{A,(T,x_{A,1})}0.75V_2 = 0$$

$$F_{A,02} - F_{A,12} + r_{A,(T,x_{A,2})}V_2 = F_{A,02}x_{A,2} + r_{A,(T,x_{A,2})}V_2 = 0$$

Note que $F_{A,01} = F_{A,02} = F_{A,0}/2$, despejando $V_2$ se obtiene

$$V_2 = \frac{-F_{A,01}x_{A,1}}{0.75r_{A,(T,x_{A,1})}} = \frac{-F_{A,02}x_{A,2}}{r_{A,(T,x_{A,2})}}$$

Además, teniendo en cuenta que

$$x_A = \frac{(F_{A,0} - F_{A,1})}{F_{A,0}} = \frac{F_{A,01} + F_{A,02} - F_{A,11} - F_{A,12}}{F_{A,01} + F_{A,02}} = \frac{F_{A,01} - F_{A,11}}{F_{A,01} + F_{A,02}} + \frac{F_{A,02} - F_{A,12}}{F_{A,01} + F_{A,02}}$$

$$x_A = \frac{F_{A,01} - F_{A,11}}{2F_{A,01}} + \frac{F_{A,02} - F_{A,12}}{2F_{A,02}} = \frac{x_{A,1} + x_{A,2}}{2}$$

Teniendo, entonces, dos ecuaciones con dos incognitas ($x_{A,1}, x_{A,2}$)

```
Obj = @(xAi) [(-xAi(1)/(0.75*rA(T0,xAi(1)))+xAi(2)/(rA(T0,xAi(2))));...
    (xAi(1)+xAi(2))/2-xA] ;
xAi = fsolve(@(x) Obj(x),[0.5;0.5])
```

```
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.

<stopping criteria details>
xAi = 2×1
    0.8312
    0.8688
```

```
xA1b = xAi(1)
```

```
xA1b = 0.8312
```

```
xA2b = xAi(2)
```

```
xA2b = 0.8688
```

```
V1b = -FA0/2*xA1b/rA(T0,xA1b) %m3
```

```
V1b = 4.0519
```

```
V2b = V1b/0.75
```

```
V2b = 5.4026
```

```
Vtotalb = V1b+V2b
```

```
Vtotalb = 9.4545
```

### C. Dos reactores PFR en serie, $V_1 = 2V_2$.

Hacemos balance de materia

$$\frac{dF_A}{dV} = r_{A(T,x_A)} \rightarrow \frac{dx_A}{dV} = -\frac{r_{A(T,x_A)}}{F_{A0}}$$

Luego,

$$V_1 = \int_0^{V_1} dV = -F_{A0} \int_0^{x_{A1}} \frac{dx_A}{r_{A(T,x_A)}}$$

$$V_2 = \int_0^{V_2} dV = -F_{A0} \int_{x_{A1}}^{x_{A2}} \frac{dx_A}{r_{A(T,x_A)}} = \frac{V_1}{2}$$

En este caso $x_{A2} = x_A$. Por tanto

$$2 \int_{x_{A1}}^{x_{A2}} \frac{dx_A}{r_{A(T,x_A)}} = \int_0^{x_{A1}} \frac{dx_A}{r_{A(T,x_A)}}$$

Donde tenemos 1 ecuación y una incognitad

```
Obj3 = @(xA1) integral(@(x) 1./rA(T0,x),0,xA1)-2*integral(@(x) 1./rA(T0,x),xA1,xA)
```

```
Obj3 = function_handle with value:
    @(xA1)integral(@(x)1./rA(T0,x),0,xA1)-2*integral(@(x)1./rA(T0,x),xA1,xA)
```

```
xA1c = fsolve(@(x) Obj3(x),0.5)
```

```
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.
```

```
<stopping criteria details>
xA1c = 0.7083
```

```
V1c =-FA0*integral(@(x) 1./rA(T0,x),0,xA1c)
```

```
V1c = 2.2104
```

```
V2c = V1c/2
```

```
V2c = 1.1052
```

```
Vtotalc = V1c+V2c
```

```
Vtotalc = 3.3156
```

## D. Dos reactores PFR en paralelo (El flujo se divide en partes iguales). $V_1 = 1.5V_2$

Hacemos balance de materia

$$\frac{dF_A}{dV} = r_{A(T,x_A)} \rightarrow \frac{dx_A}{dV} = -\frac{r_{A(T,x_A)}}{F_{A0}}$$

Luego,

$$V_1 = \int_0^{V_1} dV = -F_{A,01}\int_0^{x_{A1}} \frac{dx_A}{r_{A(T,x_A)}}$$

$$V_2 = \int_0^{V_2} dV = -F_{A,02}\int_0^{x_{A2}} \frac{dx_A}{r_{A(T,x_A)}} = 1.5V_1$$

Luego,

$$\frac{1}{1.5}\int_0^{x_{A2}} \frac{dx_A}{r_{A(T,x_A)}} = \int_0^{x_{A1}} \frac{dx_A}{r_{A(T,x_A)}}$$

Donde $F_{A,01} = F_{A,02} = F_{A,0}/2$. También se puede verificar que

$$x_A = \frac{F_{A,01} - F_{A,11}}{2F_{A,01}} + \frac{F_{A,02} - F_{A,12}}{2F_{A,02}} = \frac{x_{A,1} + x_{A,2}}{2}$$

Teniendo dos ecuaciones y dos incognitas. Resolvemos y encontramos

```
Obj4 = @(xAi) [1/1.5*integral(@(x) 1./rA(T0,x),0,xAi(2))-integral(@(x) 1./rA(T0,x),0,xAi(1));...
    (xAi(1)+xAi(2))/2-xA]
```

```
Obj4 = function_handle with value:
    @(xAi)[1/1.5*integral(@(x)1./rA(T0,x),0,xAi(2))-integral(@(x)1./rA(T0,x),0,xAi(1));(xAi(1)+xAi(2))/2-xA]
```

```
xAi = fsolve(@(x) Obj4(x),[0.5;0.5]) ;
```

```
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.
```

```
<stopping criteria details>
```

```
xA1d = xAi(1)
```

```
xA1d = 0.7902
```

```
xA2d = xAi(2)
```

```
xA2d = 0.9098
```

```
V1d = -FA0/2*integral(@(x) 1./rA(T0,x),0,xA1d)
```

```
V1d = 1.3811
```

```
V2d = -FA0/2*integral(@(x) 1./rA(T0,x),0,xA2d)
```

```
V2d = 2.0716
```

```
Vtotald = V1d + V2d
```

```
Vtotald = 3.4527
```

Registrando los resultados en la siguiente tabla

```
V1 = [Va;V1b;V1c;V1d] ;
V2 = [Va;V2b;V2c;V2d] ;
Vtotal = [Vtotala;Vtotalb;Vtotalc;Vtotald] ;
xA1 = [xA1a;xA1b;xA1c;xA1d] ;
xA2 = [xA;xA2b;xA;xA2d] ;

table(V1,xA1,V2,xA2,Vtotal,'RowNames',{'a)','b)','c)','d)'})
```

ans = 4×5 table

| | V1 | xA1 | V2 | xA2 | Vtotal |
|---|---|---|---|---|---|
| 1 a) | 2.6616 | 0.6064 | 2.6616 | 0.8500 | 5.3232 |
| 2 b) | 4.0519 | 0.8312 | 5.4026 | 0.8688 | 9.4545 |
| 3 c) | 2.2104 | 0.7083 | 1.1052 | 0.8500 | 3.3156 |
| 4 d) | 1.3811 | 0.7902 | 2.0716 | 0.9098 | 3.4527 |