

# Seminar0

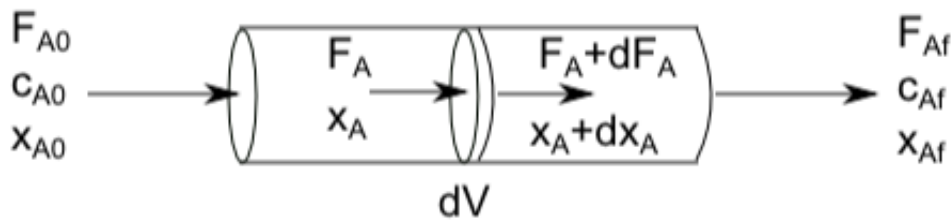
January 13, 2020

## 0.0.1 Seminar1 - Chemical Reactor Analysis II

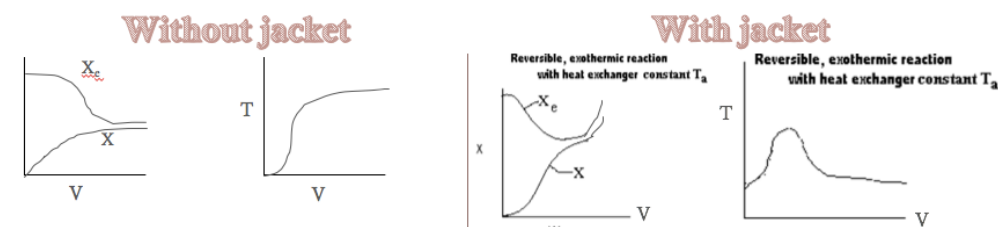
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**Q1.** For an exothermic reversible reaction occurring in an adiabatic PFR, qualitatively sketch the trends of  $X$  and  $T$  with reactor volume  $V$ . On the plot of  $X$  vs  $V$ , also indicate how the equilibrium conversion would vary with the reactor temperature. Finally, sketch how you would expect the  $X$ ,  $X_{eq}$  and  $T$  to look if a well-designed heat exchange jacket with constant temperature of coolant was added to the system.

**Answer**

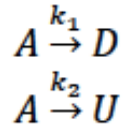


PFR.png



Q1fig.png

**Q2.** Consider a PFR with a volume of  $50\text{dm}^3$ , used to conduct a liquid phase system of reactions. If  $k_1 = 0.05\text{s}^{-1}$  and  $k_2 = 0.01\text{s}^{-1}$ ,  $C_{A0} = 1\text{mol}/\text{dm}^3$ , and the volumetric flow rate is  $50\text{dm}^3/\text{min}$ , find the outlet concentrations of A, D and U.



1.png

**Answer.**

In a liquid phase PFR.  $v_0 = 50 \frac{dm^3}{min} = \frac{50}{60} \frac{dm^3}{s}$ ,  $C_{A0} = 1 mol/dm^3$ ,  $V = 50 dm^3$

$$\frac{dF_A}{dV} = r_A = -(k_1 + k_2)C_A \quad (1)$$

$$v_0 \frac{dC_A}{dV} = r_A = -(k_1 + k_2)C_A \quad (2)$$

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = -\frac{(k_1 + k_2)}{v_0} \int_0^V dV \quad (3)$$

$$C_A = C_{A0} \exp\left(-(k_1 + k_2) \frac{V}{v_0}\right) \quad (4)$$

$$C_A = 0.0273 mol/dm^3 \quad (5)$$

```
[2]: import numpy as np
from scipy.integrate import odeint

CA0=1 #mol/dm^3
V=50 #dm^3
k1=0.05
k2=0.01

V=np.linspace(0.,50.,25)
Ca=np.zeros(len(V))

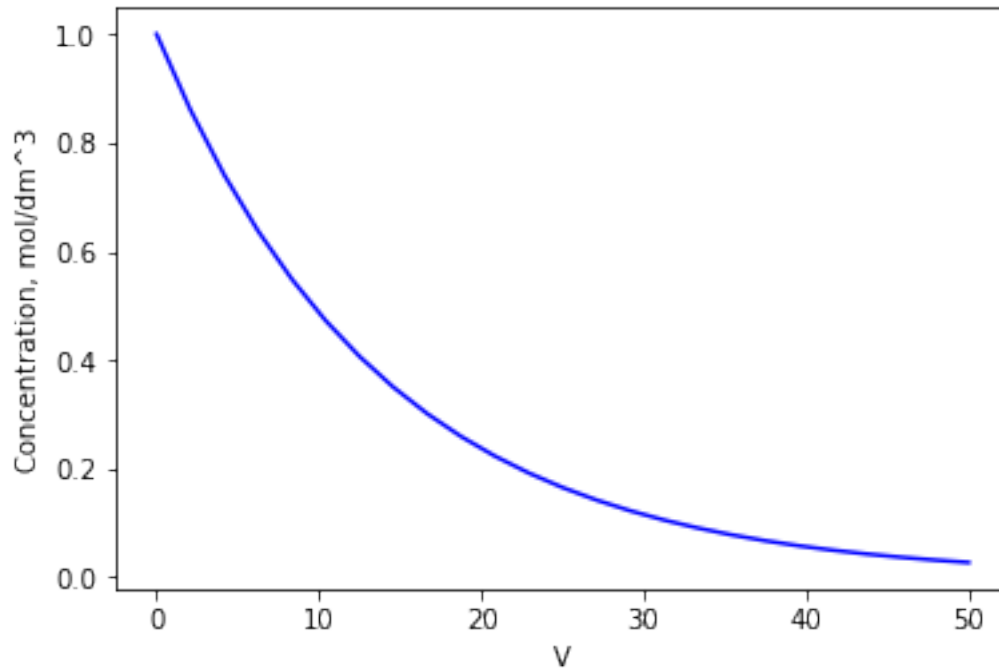
def fun(Ca,V):
    k1=0.05
    k2=0.01
    v0=50./60. #\frac{dm^3}{s}
    dcdv=-(k1+k2)/v0*Ca
    return dcdv

init_ca=1.0

Ca=odeint(fun,init_ca,V)

import matplotlib.pyplot as plt
plt.plot(V, Ca, 'b-', label='Ca(t)')
plt.xlabel('V')
plt.ylabel('Concentration, mol/dm^3')
```

[2]: Text(0, 0.5, 'Concentration, mol/dm^3')



Both species  $D$  and  $U$  have the same type of rate equations.

$$\frac{dF_D}{dV} = r_D = k_1 C_A = k_1 C_{A0} \exp\left(-(k_1 + k_2) \frac{V}{v_0}\right) \quad (6)$$

$$\frac{dF_U}{dV} = r_U = k_2 C_A = k_2 C_{A0} \exp\left(-(k_1 + k_2) \frac{V}{v_0}\right) \quad (7)$$

$$\frac{\text{mole of } D \text{ produced}}{\text{mole of } U \text{ produced}} = \frac{k_1}{k_2} = 5 \quad (8)$$

Also for every mole of  $A$  consumed, 1 total mole of products are produced.

$$C_D = (1 - 0.0273) \frac{5}{5 + 1} = 0.8106 \frac{\text{mol}}{\text{dm}^3} \quad (9)$$

$$C_U = (1 - 0.0273) \frac{1}{5 + 1} = 0.1621 \frac{\text{mol}}{\text{dm}^3} \quad (10)$$

```
[5]: k1/k2
      Ca[24]
```

```
[5]: array([0.02732372])
```

```
[6]: CD=(1-Ca[len(Ca)-1])*k1/(k1+k2)
```

```
[25]: print("CD = ", CD)
```

```
CD = [0.81056357]
```

```
[26]: CU=(1-Ca[len(Ca)-1])*k2/(k1+k2)
```

```
[27]: print("CU = ", CU)
```

CU = [0.16211271]

**Q3.** A second order gas phase reaction is conducted in an adiabatic constant volume batch reactor.  $A + B \rightarrow C$ ,  $-r_A = kC_A C_B$ ,  $k = 20 \frac{dm^3}{mol.s}$  at 400K. The initial reactor temperature is 400K, and the initial pressure is 100kPa. The volume of the reactor is 500  $dm^3$ . The reactor is charged initially with 40%A, 30%B, and 30% inerts. The constant volume heat capacity of the mixture remains constant at 50J/mol/K, and the heat of reaction is constant at  $-10kJ/mol$ . If the activation energy of the reaction  $E_a = 0$ , calculate the time to reach 50% conversion, and the temperature and pressure at this conversion.

**Answer.**

.	Initial	Final
A	$N_{A0}$	$0.5N_{A0}$
B	$0.75N_{A0}$	$0.75N_{A0} - 0.5N_{A0}$
C	0	$0.5N_{A0}$
I	$0.75N_{A0}$	$0.75N_{A0}$
Total	$2.5N_{A0}$	$2N_{A0}$

Adiabatic operating line:

$$T = T_0 + \frac{(-\Delta H_{rxn})X}{\sum \Theta_i C_{p_i}} \quad (11)$$

$$T = 400 + \frac{10,000}{50}X \text{ at } X = 0.5 \quad T = 500K \quad (12)$$

$$N_{T,0} = \frac{P_0 V}{RT} = \frac{100 \text{ kPa} * 500 \text{ dm}^3}{8.314 \frac{Pa.m^3}{mol.K} * 400 \text{ K}} = 15.03 \text{ moles} \quad (13)$$

$$\frac{N_T}{N_{T,0}} = \frac{2N_{A,0}}{2.5N_{A,0}} = 0.8 \quad (14)$$

$$P = \frac{N_T RT}{V} = \frac{15.03 * 0.8 * 8.314 * 500}{500/1000} = 10^5 Pa = 100kPa \quad (15)$$

Mole balance:

$$N_{A,0} \frac{dX}{dt} = kC_A C_B C_{A0} V \frac{dX}{dt} = kC_{A0}^2 (1-X)(\Theta_B - X) \quad (16)$$

$$\int_0^{X=0.5} \frac{dX}{(1-X)(\Theta_B - X)} = \frac{kC_{A0}}{V} \int_0^t dt = \frac{kC_{A0}t}{V} \quad (17)$$

$$\frac{kC_{A0}t}{V} = \left( \frac{\ln(1-X)}{(1-\Theta_B)} - \frac{\ln(\Theta_B - X)}{\Theta_B(1-\Theta_B)} \right)_{0 \rightarrow X=0.5} \quad (18)$$

$$C_{A0} = 0.4C_{T0} = 0.4 \frac{N_{T0}}{V} = \frac{0.4 * 15.03}{500/1000} = 3.37 \text{ s} \quad (19)$$

```
[34]: import numpy as np
```

```
P0=100 #kPa
V=500 #dm^3
R=8.314 #Pa.m^3/(mol.K)
T0=400 #K
Hrx=10000
CP=50
x=0.5 #conversion

NT0=P0*V/(R*T0)

T=T0+Hrx*x/CP
```

```
[35]: NT0
```

```
T0
```

```
[35]: 400
```

```
[ ]:
```

**Q4.** A liquid phase elementary reaction  $2A \rightarrow B$  is carried out in a CSTR with pure  $A$  in the feed. If the pre-exponential factor is  $2 * 10^3$  L/mol/min,  $E_a = 40 \text{ kJ/mol}$ ,  $C_{A0} = 1 \text{ mol/L}$ ,  $F_{A0} = 2 \text{ mol/min}$ ,  $C_p \text{ mix} = 25 \text{ J/mol/K}$  (constant),  $-\Delta H_{rxn} = 20 \text{ kJ/mol}$  (constant), and the feed temperature is  $325 \text{ K}$ , find the CSTR volume required to achieve 10% conversion in adiabatic operation. Also find the Damkohler number for this case.

**Answer.**

Adiabatic operating line, neglect  $\Delta C_p$

$$T = T_0 + \frac{(-\Delta H_{rxn})X}{\sum \Theta_i C_{p1}} \quad (20)$$

$$T = 325 + \frac{20000X}{25} = 325 + 800X \quad (21)$$

$$\text{at } X = 0.1 \quad T = 405 \text{ K} \quad K(T) = 2 * 10^3 \exp\left(\frac{-E_a}{RT}\right) = 1.386 * 10^{-2} \quad (22)$$

$$(23)$$

Molar Balance:\

$$V = \frac{f_{A0}X}{-r_A} = \frac{2 * 0.1}{(1.39 * 10^{-2})C_{A0}^2(1 - X)^2} \quad (24)$$

$$V = \frac{2 * 0.1}{(1.39 * 10^{-2})(1 - 0.1)^2} = 17.81 \text{ L} \quad (25)$$

Damkohler Number:\

$$Da = kC_{A0}\tau = (1.39 * 10^{-2}) * 1 * \frac{V}{v_0} = (1.39 * 10^{-2}) * 1 * \frac{V}{F_{A0}/C_{A0}} \quad (26)$$

$$Da = \frac{(1.39 * 10^{-2}) * 1 * 17.81}{2/1} = 0.12 \quad (27)$$

**Q5.** A constant - pressure batch reactor was charged with an equimolar feed of A and B. The reaction  $A + 2B \rightarrow C$  proceeds at 900K and 2atm. The rate law is  $-r_A = k_A C_A C_B$  with  $k_A = 0.3 \text{ Lmol}^{-1} \text{ min}^{-1}$ . What time is necessary to reach 0.005M concentration of the product?

**Answer.** B is the limiting reactant. Therefore,  $\frac{1}{2}A + B \rightarrow \frac{1}{2}C$ .

Stoichiometric Table

.	Initial	Used	Final
A	$N_{B0}$	$-0.5 N_{B0} X_B$	$N_{B0}(1 - 0.5X_B)$
B	$N_{B0}$	$-N_{B0} X_B$	$N_{B0}(1 - X_B)$
C	0	$0.5N_{B0} X_B$	$0.5N_{B0} X_B$

$$\epsilon_B = y_B \cdot \delta_B = 0.5 \left( \frac{1}{2} - \left( 1 + \frac{1}{2} \right) \right) = -0.5 \quad (28)$$

$$V = V_0(1 + \epsilon X_B) \frac{P_0}{P} \frac{T}{T_0} = V_0(1 - 0.5X_B) \quad (29)$$

$$C_A = \frac{N_A}{V} = \frac{N_{B0}(1 - 0.5X_B)}{V_0(1 - 0.5X_B) \frac{P_0}{P} \frac{T}{T_0}} = C_{B0} \frac{1 - 0.5X_B}{1 - 0.5X_B} \quad (30)$$

$$C_B = \frac{N_B}{V} = C_{B0} \frac{1 - X_B}{1 - 0.5X_B} \quad (31)$$

$$C_C = \frac{N_C}{V} = 0.5C_{B0} \frac{X_B}{1 - 0.5X_B} \quad (32)$$

$$P = P_0, \quad T = T_0 \Rightarrow C_A = C_{B0} \frac{1 - 0.5X_B}{1 - 0.5X_B} = C_{B0} \quad (33)$$

$$C_{B0} = \frac{P_{B0}}{RT} = \frac{y_{B0}P_0}{RT} = \frac{0.5 * 2}{0.082 * 900} = 0.01355 \text{ M}$$

$$C_c = 0.005 = 0.5 * 0.01355 * \frac{X_B}{1 - 0.5X_B} \Rightarrow X_B = 0.539 \quad (34)$$

Mole Balance:\

$$N_{B0} \frac{dX_B}{dt} = -r_B * V = k_B C_A C_B V = k_B C_{B0}^2 \frac{1 - X_B}{1 - 0.5X_B} V_0(1 - 0.5X_B) \quad (35)$$

$$\frac{dX_B}{dt} = \frac{C_{B0}^2}{C_{B0}} k_B (1 - X_B) \quad (36)$$

$$\int_0^{X_B} \frac{dX_B}{1 - X_B} = C_{B0} k_B t$$

$$\ln\left(\frac{1}{1 - X_B}\right) = \ln\left(\frac{1}{1 - 0.539}\right) = 0.774 \text{ and } k_B = 2k_A = 0.6 \frac{\text{L}}{\text{mol} \cdot \text{min}}$$

$$\Rightarrow t = \frac{0.774}{0.01355 * 0.6} = 95 \text{ min}$$

[ ]: