Øving 2

Den termiske spaltingen av dinitrogenoksid kan betraktes som en irreversibel, 2. ordens reaksjon:

$$2N_2O \rightarrow 2N_2 + O_2$$

Hastighetskonstanten for spaltningen av N_2O ved 895 °C er funnet å være:

$$k_{N2O} = 0.977 \text{ l/mol}\cdot\text{sek}$$

Reaksjonen utføres i flere reaktortyper ved 895 °C og en omsetningsgrad av N_2O lik 0.9.

Beregn nødvendig reaksjonstid i en satsreaktor (batchreaktor) når:

a) Volumet holdes konstant og starttrykket for N_2O er 1 atm.
b) Trykket holdes konstant lik 1 atm.

La $A = N_2O$, $B = N_2$, $C = O_2$

rx: $2A \rightarrow 2B + C$

$A \rightarrow B + \frac{1}{2}C$

$k_A = 0{,}977 \frac{L}{mol \cdot s}$

$X_A = 0{,}9$

a) Batchreaktor, konstant volum

- I: Molbalanse

$$-r_A = \frac{N_{A0}}{V}\frac{dX}{dt} = C_{A0}\frac{dX}{dt}$$

(V=konstant)

- II: Reaksjonsorden

2. ordens rx: $-r_A = k_A C_A^2$

- III: Støkiometri

$$C_A = C_{A0}(1-X)$$

- IV: Kombinerer

$$k_A C_A^2 = C_{A0}\frac{dX}{dt}$$

$$dt = \frac{C_{A0}}{k_A C_{A0}^2 (1-X)^2}\,dX$$

$$dt = \frac{1}{k_A C_{A0}}\frac{dX}{(1-X)^2}$$

$$\int_0^t dt = \frac{1}{k_A C_{A0}}\int_0^X \frac{dX}{(1-X)^2}$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$t = \frac{1}{k_A C_{A0}}\cdot\frac{X}{1-X}$$

- V: Evaluering

$$t = \frac{1}{0{,}977 \frac{L}{mol\cdot s}\cdot 0{,}01\frac{mol}{L}}\cdot\frac{0{,}9}{1-0{,}9}$$

Finner C_{A0} ved gassloven:

$$C_{A0} = \frac{N_{A0}}{V} = \frac{P}{RT} = \frac{1\,atm}{0{,}082\frac{L\cdot atm}{K\cdot mol}\cdot 1168K} = 0{,}01\frac{mol}{L}$$

$$t = 882\,s$$

b) Batchreaktor, konstant trykk

- I: Molbalanse

$$-r_A = \frac{N_{A0}}{V}\frac{dX}{dt} = \frac{N_{A0}}{V_0}\frac{1}{1+\varepsilon X_A}\frac{dX}{dt} = C_{A0}\frac{1}{1+\varepsilon X_A}\frac{dX}{dt}$$

$$V = V_0(1+\varepsilon X_A)\frac{P_0}{P}\cdot\frac{T}{T_0}$$

P og T er konstant

$$\delta = 1 + \tfrac{1}{2} - 1 = \tfrac{1}{2}$$

Inntaksstrøm er ren A

$$\Rightarrow y_{A0} = 1$$

$$\Rightarrow \varepsilon = \delta y_{A0} = \tfrac{1}{2}$$

- II: Reaksjonsorden

2. ordens rx: $-r_A = k_A C_A^2$

- III: Støkiometri

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V}$$

$$C_A = \frac{N_{A0}}{V_0}\frac{(1-X)}{(1+\varepsilon X)}$$

$$C_A = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}$$

- IV: Kombinerer

$$C_{A0}\frac{1}{1+\varepsilon X_A}\frac{dX}{dt} = k_A C_A^2 = k_A C_{A0}^2\frac{(1-X)^2}{(1+\varepsilon X)^2}$$

$$\frac{dX}{dt} = k_A C_{A0}\frac{(1-X)^2}{1+\varepsilon X}$$

$$k_A C_{A0}\,dt = \frac{1+\varepsilon X}{(1-X)^2}dX$$

$$\int_0^t k_A C_{A0}\,dt = \int_0^X \frac{1+\varepsilon X}{(1-X)^2}dX$$

$$\int_0^X \frac{1+\varepsilon X}{(1-X)^2}dX = \frac{(1+\varepsilon)X}{1-X} - \varepsilon\ln\frac{1}{1-x}$$

$$\Rightarrow t = \frac{1}{k_A C_{A0}}\left(\frac{(1+\varepsilon)X}{1-X} - \varepsilon\ln\frac{1}{1-X}\right)$$

$$t = \frac{1}{0{,}977\,\frac{L}{mol\cdot s}\cdot 0{,}1\,\frac{mol}{L}}\left(\frac{(1+0{,}5)0{,}9}{1-0{,}9} - 0{,}5\ln\frac{1}{1-0{,}9}\right)$$

$$\underline{\underline{t = 1211\text{ s}}}$$

Calculate the necessary reactor volume at constant pressure of 1 atm and a feed rate of N_2O equal to 1 mol/min for the following continuous reactor systems:

$P = P_0 = 1\ \text{atm}$

$F_A = 1\ \frac{mol}{min} = \frac{1}{60}\ \frac{mol}{s}$

c) Plug flow reactor (PFR).
d) Continuously stirred tank reactor (CSTR).

C) PFR, konstant trykk

- I: Molbalanse

$$-r_A = F_{A0}\frac{dX}{dV}$$

- II: Reaksjonsorden

2. ordens rx: $-r_A = k_A C_A^2$

- III: Støkiometri

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V}$$

$$C_A = \frac{N_{A0}}{V_0}\frac{(1-X)}{(1+\varepsilon X)}$$

$$C_A = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}$$

- IV: Kombinerer

$$F_{A0}\frac{dX}{dV} = k_A C_{A0}^2 \frac{(1-X)^2}{(1+\varepsilon X)^2}$$

$$\int_0^V dV = \frac{F_{A0}}{k_A C_{A0}^2}\int_0^V \frac{(1+\varepsilon X)^2}{(1-X)^2}\,dX$$

$$\int_0^X \frac{(1+\varepsilon X)^2}{(1-X)^2}dX = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}$$

$$V = \frac{F_{A0}}{k_A C_{A0}^2}\left(2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}\right)$$

$$V = \frac{1/60\ \frac{mol}{s}}{0{,}977\ \frac{L}{mol\cdot s}\cdot 0{,}1^2\ \frac{mol^2}{L^2}}\left(2\cdot 0{,}5(1+0{,}5)\ln(1-0{,}9) + 0{,}5^2\,0{,}9 + \frac{(1+0{,}5)^2\,0{,}9}{1-0{,}9}\right)$$

$$\underline{\underline{V = 2663\ L}}$$

d) CSTR, konstant trykk

- I: Molbalanse

$$-r_A = \frac{F_{A0} X}{V}$$

- II: Reaksjonsorden

2. ordens rx: $-r_A = k_A C_A^2$

- III: Støkiometri

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V}$$

$$C_A = \frac{N_{A0}}{V_0} \frac{(1-X)}{(1+\varepsilon X)}$$

$$C_A = C_{A0} \frac{(1-X)}{(1+\varepsilon X)}$$

- IV: Kombinerer

$$\frac{F_{A0} X}{V} = k_A C_A^2$$

$$V = \frac{F_{A0} X}{k_A C_{A0}^2} \cdot \frac{(1+\varepsilon X)^2}{(1-X)^2}$$

$$V = \frac{1/60 \frac{mol}{s} \cdot 0{,}9}{0{,}977 \frac{L}{mol \cdot s} \cdot 0{,}1^2 \frac{mol^2}{L^2}} \cdot \frac{(1 + 0{,}5 \cdot 0{,}9)^2}{(1-0{,}9)^2}$$

$$\underline{\underline{V = 29611 \text{ L}}}$$