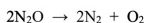


Øving 2

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



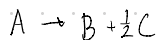
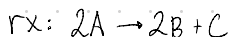
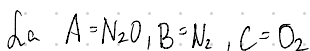
Hastighetskonstanten for spaltningen av N_2O ved 895°C er funnet å være:

$$k_{\text{N}_2\text{O}} = 0.977 \text{ l/mol}\cdot\text{sek}$$

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.



$$k_A = 0.977 \frac{\text{l}}{\text{mol}\cdot\text{s}}$$

$$X_A = 0.9$$

a) Batchreaktor, konstant volum

• I: Molbalanse

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

• II: Reaksjonsorden

$$2. \text{ ordens rx: } -r_A = k_A C_A^2$$

• III: Støkiometri

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

• IV: Kombinerer

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

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

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

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

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

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

• V: Evaluering

$$t = \frac{1}{0.977 \frac{\text{l}}{\text{mol}\cdot\text{s}} \cdot 0.01 \frac{\text{mol}}{\text{l}}} \cdot \frac{0.9}{1-0.9}$$

$$\underline{t = 882 \text{ s}}$$

Finner C_{A0} ved gassloven:

$$C_{A0} = \frac{N_{A0}}{V} = \frac{P}{RT} = \frac{1 \text{ atm}}{0.082 \frac{\text{l}\cdot\text{atm}}{\text{mol}\cdot\text{K}} \cdot 1168 \text{ K}} = 0.01 \frac{\text{mol}}{\text{l}}$$

b) Batchreaktor, konstant trykk

• I: Molbalanse

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

• II: Reaksjonsorden

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

• III: Støkiometri

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

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

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

• IV: Kombinerer

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

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

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

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

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

$$t = \frac{1}{0.977 \frac{\text{L}}{\text{mol} \cdot \text{s}} \cdot 0.1 \frac{\text{mol}}{\text{L}}} \left(\frac{(1+0.5)0.9}{1-0.9} - 0.5 \ln \frac{1}{1-0.9} \right)$$

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

$$V = V_0 (1 + EX_A)^{\frac{P_0}{P}} \frac{T}{T_0}$$

P og T er konstant

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

Inntaksstrøm er ren A

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

$$\Rightarrow \epsilon = \delta y_{A0} = \frac{1}{2}$$

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

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:

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

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

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

$$2. \text{ordens rx: } -r_A = k_A C_A^2$$

• III: Støkiometri

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

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

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

• IV: Kombinerer

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

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

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

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

$$V = \frac{1/60 \frac{\text{mol}}{\text{s}}}{0.977 \frac{\text{K}}{\text{mol} \cdot \text{g}} \cdot 0.1^2 \frac{\text{mol}^2}{\text{L} \cdot \text{g}}} \left(2 \cdot 0.5(1+0.5)\ln(1-0.9) + 0.5^2 \cdot 0.9 + \frac{(1+0.5)^2 \cdot 0.9}{1-0.9} \right)$$

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

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

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

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

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

• IV: Kombinerer

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

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

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

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