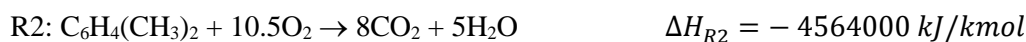
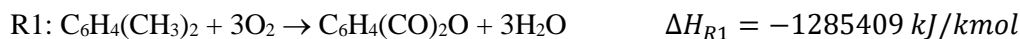


Practical 9

1D+1D Pseudo Homogeneous Model

Exercise 1

Phthalic Anhydride (PA) is industrially produced by the oxidation of the o-xylene on $V_2O_5 - TiO_2$ catalyst. The o-xylene diluted in air is fed to a multi tubular fixed bed reactor cooled by the circulation of a molten salts. Details of the configuration, catalysts, and operating conditions are given below. The reaction network is given by the following three reactions:



The system can be considered a mixture of ideal gases. Adopting a 1D+1D pseudo homogeneous model with the heat transfer computed through the Dixon-Specchia correlation, assess:

- 1) the number of tubes needed considering the constraints reported in the data.
- 2) the thermal profile along the tube.
- 3) the conversion of $C_6H_4(CH_3)_2$ and the selectivity of $C_6H_4(CO)_2O$ along the tube.

Data:

Reaction kinetics (R in J/mol/K, partial pressures in bar, reaction rate in kmol/kg_{cat}/h):

$$r_1 = \exp\left(19.837 - \frac{13636}{T}\right) p_{C_6H_4(CH_3)_2} p_{O_2}$$

$$r_2 = \exp\left(18.970 - \frac{14394}{T}\right) p_{C_6H_4(CH_3)_2} p_{O_2}$$

$$r_3 = \exp\left(20.860 - \frac{15803}{T}\right) p_{C_6H_4(CO)_2O} p_{O_2}$$

Operating conditions:

Maximum allowable pressure drops: 0.1 bar/m

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Outlet pressure = 1 atm

Feed Temperature = 335 °C

Diluted conditions: o-xylene to air ratio (v/v) 1.1%

Specific inlet mass flowrate (G) = 4900 kg/h/m²

Molten Salts Temperature = 335 °C

Diffusion coefficients:

N₂ = 8.31e-5 m²/s

O₂ = 7.02 e-5 m²/s

O-xylene = 2.58 e-5 m²/s

Phthalic anhydride = 2.22 e-5 m²/s

H₂O = 8.98 e-5 m²/s

CO₂ = 2.02 e-5 m²/s

Tubes:

Length = 3 m

Tube diameter = 2.54 cm

Catalyst:

Sphere diameter = 0.005 m

Catalyst density = 2100 kg/m³

$$\text{void fraction} = 0.363 + 0.35 \exp\left(-0.39 \frac{d_{\text{tube}}}{d_{\text{sphere}}}\right)$$

Particle porosity = 0.3

Particle tortuosity = 5

Pore diameter = 10 nm

Mixture properties:

Specific heat of the mixture = 0.992 kJ/kg/K

Viscosity: $2.95 \cdot 10^{-5}$ Pa s

Ergun equation:

$$\frac{\Delta P}{L} = 150 \frac{(1 - \varepsilon)^2}{\varepsilon^3} \frac{\mu v_g}{d_p^2} + 1.75 \frac{(1 - \varepsilon)}{\varepsilon^3} \frac{\rho v_g^2}{d_p}$$

Dixon – Specchia correlation:

$$\lambda_{static} = \lambda \left(\varepsilon + \frac{(1 - \varepsilon)}{\left(0.22 \varepsilon^2 + \frac{2}{3} \frac{\lambda}{\lambda_{cat}} \right)} \right)$$

$$Pe_{ref} = 8.65 \left(1 + 19.4 \left(\frac{d_p}{d_t} \right)^2 \right)$$

$$\lambda_{dynamic} = \lambda \left(Re \frac{Pr}{Pe_{ref}} \right)$$

$$\lambda_{eff} = \lambda_{static} + \lambda_{dyn}$$

$$static = 2\varepsilon + \frac{(1 - \varepsilon)}{0.0024 \left(\frac{d_t}{d_p} \right)^{1.58} + \frac{1}{3} \frac{\lambda}{\lambda_{cat}}}$$

$$\alpha_{wstatic} = static * \frac{\lambda}{d_p}$$

$$\alpha_{wdynamic} = \frac{\lambda}{d_p} 0.0835 Re^{0.91} \quad \text{if } Re < 1200$$

$$\alpha_{wdynamic} = \frac{\lambda}{d_p} 1.23 Re^{0.53} \quad \text{if } Re \geq 1200$$

$$\alpha_w = \alpha_{wdynamic} + \alpha_{wstatic}$$

$$Bi = \alpha_w \frac{d_t}{\lambda_{eff}}$$

$$A = 6 \frac{(Bi + 4)}{(Bi + 3)}$$

$$\text{Internal heat coefficient} = \frac{\alpha_w}{\left(1 + \frac{Bi}{A} \right)}$$

$$Re = \frac{\rho v_0 d_p}{\mu}$$

$$Pr = \frac{\mu C_p}{\lambda}$$

Yoshida correlation:

$$j_m = 0.61 Re_{particle}^{-0.41} \quad \text{with} \quad Re_{particle} = \frac{G d_{particle}}{6 \mu (1-\varepsilon)}$$