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:

R1: $C_6H_4(CH_3)_2 + 3O_2 \rightarrow C_6H_4(CO)_2O + 3H_2O$ $\quad \Delta H_{R1} = -1285409\ kJ/kmol$

R2: $C_6H_4(CH_3)_2 + 10.5O_2 \rightarrow 8CO_2 + 5H_2O$ $\quad \Delta H_{R2} = -\ 4564000\ kJ/kmol$

R3: $C_6H_4(CO)_2O + 7.5O_2 \rightarrow 8CO_2 + 2H_2O$ $\quad \Delta H_{R3} = -\ 3278591\ kJ/kmol$

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

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/m^2

Molten Salts Temperature = 335 °C

Diffusion coefficients:

N_2 = 8.31e-5 m^2/s

O_2 = 7.02 e-5 m^2/s

O-xylene = 2.58 e-5 m^2/s

Phthalic anhydride = 2.22 e-5 m^2/s

H_2O = 8.98 e-5 m^2/s

CO_2 = 2.02 e-5 m^2/s

Tubes:

Length = 3 m

Tube diameter = 2.54 cm

Catalyst:

Sphere diameter = 0.005 m

Catalyst density = 2100 kg/m^3

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

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 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:

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

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

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

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

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

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

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

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

$$\alpha_w = \alpha_{w_{dynamic}} + \alpha_{w_{static}}$$

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

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

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

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

$$\mathrm{Pr} = \frac{\mu Cp}{\lambda}$$

Yoshida correlation:

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

