Ch E 345 - Chemical Reactor Analysis 1
Seminar #10

April 7, 2017

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1. An irreversible first order liquid phase reaction is conducted in a CSTR. The liquid density is 1000 kg/m^3 and the liquid heat capacity is a constant 4000 J/kg·K. The volumetric flow rate is 2×10^{-4} m^3/s and the reactor volume is 0.01 m^3. The inlet temperature is 300 K and the inlet concentration of A is 1000 mol/m^3. The reaction rate is given by:

$$(-r_\mathrm{A}) = 2\times10^6\ \exp\left(\frac{-6{,}000}{T}\right) C_\mathrm{A} \quad \frac{\mathrm{mol}}{\mathrm{m^3 s}}$$

The enthalpy change of reaction is a constant : $(-\Delta H_{R,\mathrm{A}}) = 2\times10^5\ \dfrac{\mathrm{J}}{\mathrm{mol}}$. Determine the outlet conversion and temperature at steady state if the reactor is adiabatic.

2. A liquid phase reaction is conducted in a CSTR. The reaction is:

$$\mathrm{A} \rightarrow \mathrm{B} \quad \text{the reaction rate is} \quad (-r_\mathrm{A}) = k\,C_\mathrm{A}$$

The reactor operates at steady state. The following data are available:

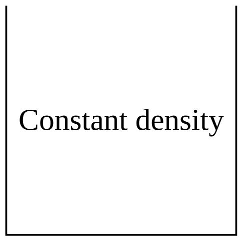
Total inlet mass flow rate	$100\ \dfrac{\mathrm{kg}}{\mathrm{s}}$	Density of feed	$1000\ \dfrac{\mathrm{kg}}{\mathrm{m^3}}$
Heat capacity of stream	$4000\ \dfrac{\mathrm{J}}{\mathrm{kg\cdot K}}$	Activation energy of reaction	$50\ \dfrac{\mathrm{kJ}}{\mathrm{mol\cdot K}}$
Heat of reaction	$-10\ \dfrac{\mathrm{kJ}}{\mathrm{mol}}$	Pre-exponential factor	$25{,}000\ \mathrm{s^{-1}}$
Molar mass of A and B	$25\ \dfrac{\mathrm{g}}{\mathrm{mol}}$	Conversion in reactor of A	0.90
Mass fraction of A in feed (remainder inert)	0.50	Temperature in reactor	353 K
Inlet feed temperature	300 K	Overall heat transfer coefficient	$100\ \dfrac{\mathrm{W}}{\mathrm{m^2 K}}$

The reactor is cylindrical in shape. The height of the liquid in the reactor is equal to the reactor diameter. Heat transfer occurs through the side walls of the reactor only. Calculate the following:

a) The reactor volume.
b) The temperature of the heat transfer fluid.
c) The total heat transfer rate between the reactor fluid and the heat exchange fluid.

Solution to problem 1

Adiabatic steady state CSTR.



$V = 0.01 \text{ m}^3$

$\rho = 1000 \quad C_P = 4000$

$Q = 2 \times 10^{-4} \ \dfrac{\text{m}^3}{\text{s}}$

$C_{\text{A0}} = 1000 \ \dfrac{\text{mol}}{\text{m}^3}$

<u>Mole Balance</u>:

$$\frac{V}{F_{\text{A0}}} = \frac{X_{\text{A}}}{(-r_{\text{A}})} = \frac{\text{X}_{\text{A}}}{2 \times 10^{-6} \exp\left(\dfrac{-6000}{T}\right) C_{\text{A}}}$$

<u>Energy Balance</u> (adiabatic CSTR)**:**

$$(\dot{m} C_P)_0 \left(T_0 - T_f\right) + (-\Delta H) F_{\text{A0}} X_{\text{A}} = 0$$

C_P and ΔH are constant. In terms of Q:

$$(Q \rho C_P)_0 \left(T_0 - T_f\right) + (-\Delta H) Q C_{\text{A0}} X_{\text{A}} = 0$$

<u>Substitute</u>:

$$(1000)(4000)\left(300 - T_f\right) + \left(2 \times 10^5\right)(1000) X_{\text{A}} = 0$$

$$T_f = 300 + 50 X_{\text{A}}$$

Substitute into mole balance:

$$\frac{0.01}{\left(2 \times 10^{-4}\right)(1000)} = \frac{X_{\text{A}}}{2 \times 10^{-6} \exp\left(\dfrac{-6000}{300 + 50 X_{\text{A}}}\right) 1000 \left(1 - X_{\text{A}}\right)}$$

Solve for $X_{\text{A}} = 0.4645$.

Solution to problem 2

a) The reactor is a CSTR.

$$\mathrm{A} \rightarrow \mathrm{B} \qquad \left(-r_{\mathrm{A}}\right) = k\,C_{\mathrm{A}}$$

The rate constant is computed using the Arrhenius equation. The reactor temperature is known.

$$k = A\exp\left(-\frac{E}{R_8 T}\right) = 25{,}000\ \exp\left(\frac{\text{-50,000}}{8.314*353}\right) = 9.98\times10^{-4}\,s^{-1} \approx 1\times10^{-3}\,s^{-1}$$

The mole balance equation is:

$$V = \frac{F_{\mathrm{A0}}X_{\mathrm{A}}}{kC_{\mathrm{A0}}\left(1-X_{\mathrm{A}}\right)} = \frac{Q\,C_{\mathrm{A0}}X_{\mathrm{A}}}{k\,C_{\mathrm{A0}}\left(1-X_{\mathrm{A}}\right)}$$

The volumetric flow rate is:

$$Q = \frac{\dot{m}_t}{\rho} = \frac{100\ \frac{\mathrm{kg}}{\mathrm{s}}}{1000\frac{\mathrm{kg}}{\mathrm{m}^3}} = 0.1\ \frac{\mathrm{m}^3}{\mathrm{s}}$$

Therefore, the reactor volume is:

$$V = \frac{(0.1)(0.9)}{\left(1\times10^{-3}\right)(1-0.9)} = 900\ \mathrm{m}^3$$

b) The energy balance equation is:

$$\dot{m}_t C_P\left(T_E - T_o\right) = UA\left(T_\infty - T_E\right) = \left(-\Delta H\right)F_{\mathrm{A0}}X_{\mathrm{A}}$$

The inlet molar flowrate is:

$$F_{\mathrm{A0}} = 0.5\ \frac{\dot{m}_t}{M_{\mathrm{A}}} = \frac{0.5\left(100\ \frac{\mathrm{kg}}{\mathrm{s}}\right)}{25\times10^{-3}\ \frac{\mathrm{kg}}{\mathrm{mol}}} = 2000\ \frac{\mathrm{mol}}{\mathrm{s}}$$

The heat transfer area is the reactor side only.

$$V = \pi R^2 L = 2\pi R^3$$

The reactor radius is therefore 5.23 m. The heat transfer area is:

$$A = 2\pi RL = 4\pi R^2 = 344\ \mathrm{m}^2$$

Substitute the known values into the energy balance:

$$(100)(4000)(353-300) = (100)(344)(T_\infty - 353) + (10{,}000)(2000)(0.9)$$

Solve for $T_\infty = 446 \text{ K}$.

b) The heat transfer rate is:

$$q = UA(T_\infty - T_E) = (100)(344)(446-353) = 3{,}199{,}200 \text{ W} \equiv 3.2 \text{ MW}$$