CONTINUOS ASSESSMENT TEST - ANSWERS

Solutions.

Problem 1.

a) For first-order reaction kinetics

$$\mathrm{X_A} = \frac{\mathrm{Da}}{1+\mathrm{Da}} = \frac{\mathrm{k}\tau}{1+\mathrm{k}\tau} = \frac{2.5\times10^{-3}\ \mathrm{min}^{-1}\times\dfrac{10000L}{0.3L/\mathrm{sec}}}{1+2.5\times10^{-3}\ \mathrm{min}^{-1}\times\dfrac{10000L}{0.3L/\mathrm{sec}}} = 0.58$$

b) Consider the non-steady state design equation for CSTR, where we can have

$$\mathrm{F_{A0}} - \mathrm{F_A} + \mathrm{r_A}V = \frac{\mathrm{dN_A}}{\mathrm{dt}}$$

Since in liquid phase with constant density, we have

$$\mathrm{C_{A0}} - \mathrm{C_A} - \mathrm{kC_A}\tau = \tau\frac{\mathrm{dC_A}}{\mathrm{dt}}$$

or equivalently

$$\frac{\mathrm{dC_A}}{\mathrm{dt}} + \frac{1+\mathrm{k}\tau}{\tau}\mathrm{C_A} = \frac{\mathrm{C_{A0}}}{\tau}$$

with the initial conditions $C_{A,t=0}$=(1-0.58)×0.12 mol/L=0.05 mol/L, new τ=10000L/(0.7×0.3*60 L/min)=793.7 min

Therefore, integrate this equation we can have

$$\mathrm{C_A}(t) = \frac{\mathrm{C_{A0}}}{1+\mathrm{k}\tau}\{1-\exp[-\frac{1+\mathrm{k}\tau}{\tau}t]\} + \mathrm{C_{A,t=0}}\exp(-\frac{1+\mathrm{k}\tau}{\tau}t)$$

Therefore the conversion at time t is

$$\mathrm{X_A}(t) = 1 - \frac{1}{1+\mathrm{k}\tau}\{1-\exp[-\frac{1+\mathrm{k}\tau}{\tau}t]\} - \frac{\mathrm{C_{A,t=0}}}{\mathrm{C_{A0}}}\exp[-\frac{1+\mathrm{k}\tau}{\tau}t]$$

After 60 min of changing flow rate,

$$\mathrm{X_A}(60\,\mathrm{min}) = 1 - \frac{1}{1+\mathrm{k}\tau}\{1-\exp[-\frac{1+\mathrm{k}\tau}{\tau}t]\} - \frac{\mathrm{C_{A,t=0}}}{\mathrm{C_{A0}}}\exp[-\frac{1+\mathrm{k}\tau}{\tau}t] = 0.598$$

The new steady state fractional conversion is

$$\mathrm{X_A} = \frac{\mathrm{Da}}{1+\mathrm{Da}} = \frac{\mathrm{k}\tau}{1+\mathrm{k}\tau} = \frac{2.5\times10^{-3}\ \mathrm{min}^{-1}\times\dfrac{10000L}{0.3L/\mathrm{sec}\times0.7}}{1+2.5\times10^{-3}\ \mathrm{min}^{-1}\times\dfrac{10000L}{0.3L/\mathrm{sec}\times0.7}} = 0.665$$

c) The steady state productivity (moles/time) of B is F_B, and the ratio of that in b) vs. that in a) is

$$\frac{\mathrm{F_{B,b}}}{\mathrm{F_{B,a}}} = \frac{0.3\mathrm{L/sec}\times0.7\times0.665}{0.3\mathrm{L/sec}\times0.58} = 0.803$$

Therefore, the productivity will be decreased by lowering the flow rate even though a higher conversion is to be achieved.

Problem 2.

We know for first order reaction, conversion X_A has the following relation with rate constant k, CSTR reactor volume V and volumetric flow rate v

$$X_A = \frac{k\frac{V}{v}}{1+k\frac{V}{v}}$$

When we have a dead volume (denoted as subscript 1) which does not interact with the input and output streams, we can deduce this amount of volume from the overall reactor volume.

$$X_{A1} = \frac{k\frac{V_1}{v}}{1+k\frac{V_1}{v}}$$

We are told V_1=600L-400L=200L, X_{A1}=0.75, therefore we can calculate $\frac{k}{v} == \frac{X_{A1}}{V_1(1-X_{A1})}$=0.015.

Then for the well-stirred reactor, V=600L

$$X_A = \frac{k\frac{V}{v}}{1+k\frac{V}{v}} = 0.9$$

Problem 3.

For a PFR reactor, the design equation is

$$\frac{dX_{\text{celluose}}}{dz} = S\frac{-r_{\text{celluose}}}{F_{\text{celluose, in}}}$$

Now S=10cm^2, length=2m, $F_{\text{celluose, in}}=v_{\text{in}}[\text{cellulose}]_{\text{in}}$, in order to know v, we have to convert 60 grams of slurry into total moles of cellulose and water per second, that is

$$\dot{n}_{\text{total, in}} = \frac{60\ \text{gram/sec} \times 20\%}{MW_{\text{cellulose}}} + \frac{60\ \text{gram/sec} \times (1-20\%)}{MW_{\text{water}}} =$$

$$= \frac{60\ \text{gram/sec} \times 20\%}{720\ \text{gram/mol}} + \frac{60\ \text{gram/sec} \times (1-20\%)}{18\ \text{gram/mol}} = 2.683\ \text{mol/sec}$$

Using ideal gas law to get the volumetric flow rate:

$$v_{\text{in}} = \frac{\dot{n}_{\text{total, in}} RT}{P} = \frac{2.683\ \text{mol/sec} \times 8.314\ \text{J/mol/K} \times 600\text{K}}{20\ \text{atm}} = 6.61\ \text{liter/sec}$$

Also

$$[\text{cellulose}]_{\text{in}} = \frac{y_{\text{cellulose},0} P}{RT} = \frac{\dfrac{20\%}{720\ \text{gram/mol}}}{\left(\dfrac{20\%}{720\text{gram/mol}} + \dfrac{1-20\%}{18\text{gram/mol}}\right)} \frac{20\ \text{atm}}{8.314\text{J/(mol K)} \times 600\text{K}} = 2.52\ \text{mol/m}^3$$

where $y_{\text{cellulose},0}$ is the molar fraction of cellulose in the inlet.

In this problem, since the gas phase reaction creates more molecules, the volumetric flow rate is not a constant.

$$-r_{\text{celluose}} = k\frac{[\text{cellulose}]}{1 + a[\text{CO}]}$$

where the concentrations should be expressed (constant pressure and temperature are assumed)

$$[\text{cellulose}] = [\text{cellulose}]_{\text{in}} \frac{(1-X)}{(1+\varepsilon X)}$$

and

$$[\text{CO}] = [\text{H}_2] = [\text{cellulose}]_{\text{in}} \frac{24X}{(1+\varepsilon X)}$$

Here ε=(24+24-1)$y_{\text{cellulose},0}$=47*0.0062=0.292.

Now the final molar flow rate of H_2 is

$v_{\text{final}}[H_2]=24v_{\text{in}}[\text{cellulose}]_{\text{in}}X_f$