Solutions.

Problem 1.

a) For first-order reaction kinetics

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

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

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

Since in liquid phase with constant density, we have

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

or equivalently

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

with the initial conditions $C_{A,t=0}=(1-0.58)\times0.12$ 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

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

Therefore the conversion at time t is

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

After 60 min of changing flow rate,

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

The new steady state fractional conversion is

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

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

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

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

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

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.

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

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

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

Problem 3.

For a PFR reactor, the design equation is

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

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

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

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

Using ideal gas law to get the volumetric flow rate:

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

Also

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

where $y_{cellulose,0}$ 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.

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

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

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

and

$$[CO] = [H_2] = [cellulose]_{in} \frac{24X}{(1+\varepsilon X)}$$

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

Now the final molar flow rate of H$_2$ is

v_{final}[H$_2$]=24v_{in}[cellulose]$_{in}$X$_f$