ME 575: Project 1

The fuel for the USS Enterprise is produced in a very delicate reversible reaction. You are currently being assigned to design a reactor and separator unit to optimize production and maximize profits for the first year of operation. You will need to determine the size of a Continuously Stirred Tank Reactor (CSTR), as well as the concentration of the exit stream in order to determine the separator requirements and cost. The reactants involved are highly classified and not currently disclosed to engineering design teams; however, all necessary material properties for species A and B are provided below. Profits are determined from the sales of the product minus the principal cost of equipment, along with the cost of reactant materials. Good luck! The safety of the universe depends on your success!

The reaction proceeds as follows:

$$2A + 3B \leftrightarrow \text{Fuel}$$

The following specifications are given,

Ideal Gas Constant	R	= 8.31446 J/mol*K
Activation Energy of Desirables	E_1	= 1700 J/mol
Activation Energy of Undesirables	E_2	= 20000 J/mol
Rate pre-factor of Undesirables	A_1	= 330 m^3/mol*s
Rate pre-factor of Desirables	A_2	= 10 /s
Molecular Weight of Species A	MW_a	= 44.053 gm/mol
Molecular Weight of Species B	MW_b	= 38 gm/mol
Molecular Weight of Species C	MW_c	= 82.053 gm/mol
Density of Species A	ρ_a	= 780 g/mol
Density of Species B	ρ_b	= 700 g/mol
Density of Species C	ρ_c	= 690 g/mol
Cost of Species A		= 5 $/m^3
Cost of Species B		= 1 $/m^3
Sale price of Species C		= 6.6 $/m^3
Length of time		= 1 year

The following must be determined:

T = Temperature of Reaction (Kelvin)

F_{A0} = Initial Molar Flow rate of species A (mol/s)

F_{B0} = Initial Molar Flow rate of species B (mol/s)

X_A = Conversion Factor of reactant A (unitless)

Total profit from the plant is equal to the sales of the product minus initial costs (Reactor & Separator cost) minus operating costs (Reactants and Heating).

$$\textbf{Profits} = \textbf{Sales} - \textbf{Cost}_{Reactor} - \textbf{Cost}_{Seperator} - \textbf{Cost}_{SpeciesA} - \textbf{Cost}_{SpeciesB} - \textbf{Cost}_{Temp}$$

The cost of heating ($Cost_{Temp}$) is estimated by the temperature needed for the reaction times your total volumetric flow out times the reactor size.

$$\textbf{Cost}_{Temp} = \textbf{Temp} * \textbf{(Volume Reactor)} * \textbf{(Volumetric flow rate out)(\$)}$$

The cost of each species can be determined from the volumetric flow rate of each inlet stream. Volumetric flow is given by the following:

$$V = \frac{Fo*MW}{\rho}$$

Reactor Cost is determined as a function of the Volume of the Reactor (Vr) in m^3:

$$\textbf{Cost}_{reactor} = 9000 * V_r$$

You should note that the Volume of your reactor cannot be less than the entrance volumetric flow rate.

Volume for a Steady State CSTR can be determined from the following equation:

$$F_{A,0} - F_A + r_A V_r = 0$$

The Reaction Rate (r_A) is a combination of both forward and reverse reactions, as given in the following relation:

$$r_A = -k_1 C_A^2 C_B^3 + k_2 C_C$$

The concentrations of the reactants is a simple function of the flow rate of species x divided by the volumetric flow rate.

$$C_x = \frac{Fx}{V}$$

Take note that this is a liquid-phase reaction, and volumetric flow rates are constant. This means that $V=V_0$.

The flow rates can be determined from the following stoichiometric Table:

$$F_A = F_{A0} - F_{A0}X$$

$$F_B = F_{B0} - 3/2F_{A0}X$$

$$F_C = F_{C0} + 1/2F_{A0}X$$

$$F_T = F_{T0} - 2F_{A0}X$$

No recycle stream will be utilized, hence, flow of product entering the reactor (F_{C0}) is equal to zero. This allows us to determine our volumetric flow rate (V) by adding the two initial flow rates, A and B, multiplied by their molecular weights and divided by their respective densities. Since V = V_0, this gives us:

$$\mathbf{V_0 = \frac{F_{A0}MW_A}{\rho_A} + \frac{F_{B0}MW_B}{\rho_B}}$$

Rate constants for a reaction are functions of temperature. With increasing temperature, the rate constants increase, causing the reaction to increase. Each rate constant can be calculated respectively by the given equation:

$$\mathbf{k = Ae^{-E/RT}}$$

where

A = Rate pre-exponential factor

E = Activation Energy (J/mol)

R = Ideal Gas Constant (J/mol*K)

T = Temperature (K)

The reactants become unstable and self combustible if the temperature exceeds 500 K. They are also sensitive to cold and can become nonreactive if temperature drops lower than 350 K.

The Separator for the process is needed to remove the Fuel from the leftover reactants. Another top secret government agency is in charge of developing the Separator, but they need the fraction of Fuel in the mixture, as well as the volumetric flow rate in order to determine the cost of the Separator. They have provided you with the following equation:

$$\mathbf{Cost_{Separator} = (Total\ Volumetric\ Flow\ rate) * e^{9.24*(Fraction\ of\ Fuel)}}$$

The percent of Fuel in the mixture can be determined by dividing the molar flow rate of Fuel by the total molar flow rate.

$$\mathbf{Fraction\ of\ Fuel = \frac{Fc}{Ft}}$$

The maximum flow rate available is 100000 mol/s for each reactant. Conversion cannot exceed 100%.