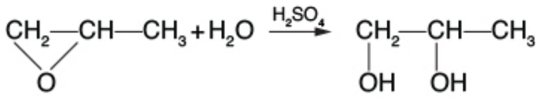
Problem 1

You are in charge of the production of propylene glycol in a batch reactor:



$$A + B \longrightarrow C$$

You are considering the installation of a new glass-lined 1000-L CSTR, and you decide to make a quick check of the reaction kinetics and maximum adiabatic temperature. For your preliminary study, you decide to use a 40-L stirred batch reactor. You charge this reactor with 4 L of ethylene oxide, 4 L of methanol, and 10 L of water containing 0.1 wt % H_2SO. At this time of year in Switzerland, the initial temperature of all materials is 13°C. If the reactor temperature increases above 77°C, a secondary, more exothermic reaction will take over, causing runaway and subsequent explosion.

You purchased some low quality data from the web for this reaction. The values you purchased were :

E_a **= 1800 cal/mol**

ΔH_R° **= -20202 cal/mol**

c_{p_A} **= 35 cal/mol/K**

c_{p_B} **= 18 cal/mol/K**

c_{p_C} **= 46 cal/mol/K**

c_{p_M} **= 19.5 cal/mol/K**

The initial concentrations of pure propylene oxide and methanol are 13.7 and 24.7 mol/dm³, respectively. Consequently, the initial number of moles added to the reactor are :

A: propylene oxide: N_{A0} **= (13.7 mol/L * 4 L) = 54.8 mol**

B: Water: N_{B0} **= (55.5 mol/L * 10 L) = 555 mol**

M: méthanol: N_M **= (24.7 mol/L * 4 L) = 98.8 mol**

The sulfuric acid catalyst takes up negligible space, so the total volume is 18 L.

Here are some additional data :

$k = 2.73 \cdot 10^{-4} \cdot \exp\left(9059 \cdot \left(\frac{1}{297} - \frac{1}{T}\right)\right)$ 1/s

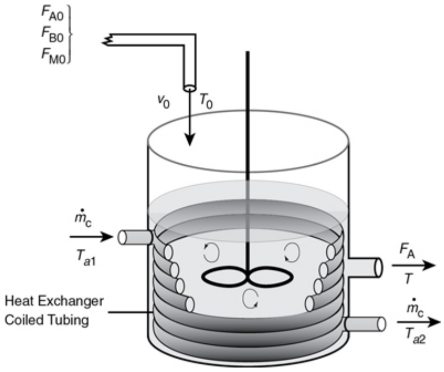
Avec

$r = k \cdot C_A$ (B is present in large excess and does not participate to the reaction kinetics)

We are going to carry out two scenarios: (1) to learn how fast the temperature rises and how long it takes to reach 350 K for adiabatic operation, and (2) how long would it take to reach 345 K if we added a heat exchanger.

1. **Adiabatic Operation:** Plot conversion and temperature *X* and *T* as a function of time for adiabatic operation. How many minutes should it take the mixture inside the reactor to reach a conversion of 51.5%? What is the corresponding adiabatic temperature?
2. **Heat Exchange:** Plot the temperature and conversion as a function of time when a heat exchanger is added. The product of the overall heat transfer coefficient and exchange surface area is *UA* = 10 cal/s/K with T_{a1} = 290 K and the coolant rate is 10 g/s, and it has a heat capacity of 4.16 cal/g/K.

Problem 2



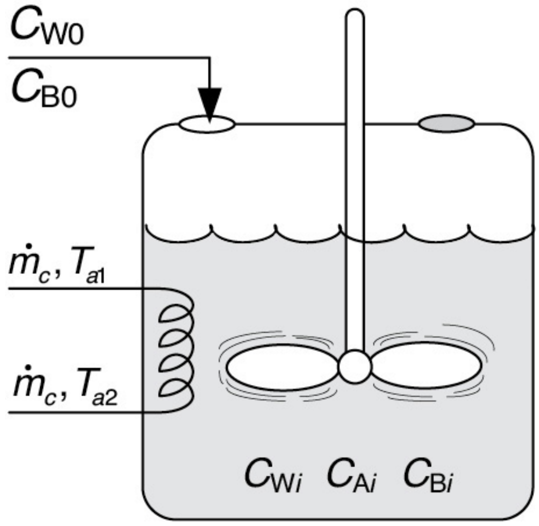
Again, we consider the production of propylene glycol (C) in a CSTR with a heat exchanger. Initially there is only water, C_{wi} = 55.3 kmol/m³, at T_i = 297 K and 0.1 wt % H_2SO_4 in the 1.89 m³ reactor. The feed stream consists of 36.3 kmol/h of propylene oxide (A), 453.6 kmol/h of water (B) containing 0.1 wt % H_2SO_4, and 45.4 kmol/h of methanol.

The water coolant flows through the heat exchanger at a rate of 2.27 kg/s (453.6 kmol/h). The molar densities of pure propylene oxide (A), water (B), and methanol (M) are ρ_{A0} = 14.8 kmol/m³, ρ_{B0} = 55.3 kmol/ m³, and ρ_{M0} = 24.7 kmol/ m³, respectively.

Plot the temperature and concentration of propylene oxide as a function of time, and also the concentration of A as a function of temperature for different entering temperatures and initial concentrations of A in the reactor to learn whether the practical stability limit of 355 K is exceeded.

UA is 7262 kcal/h/K in this reactor.

Problem 3



The second-order saponification of ethyl acetate is to be carried out in a semibatch reactor shown schematically in the figure above.

$$C_2H_5\,(CH_3COO)\,(aq) + NaOH(aq) \leftrightarrows Na\,(CH_3COO)(aq) + C_2H_5\;OH(aq)$$
$$A \;+\; B \;\leftrightarrows\; C \;+\; D$$

Aqueous sodium hydroxide is to be fed at a concentration of 1 kmol/m³, a temperature of 300 K, and a volumetric rate of 0.004 m³/s to an initial volume of 0.2 m³ of water and ethyl acetate. The concentration of water in the feed, C_{W0}, is 55 kmol/m³. The initial concentrations of ethyl acetate and water in the reactor are 5 and 30.7 kmol/m³, respectively. The reaction is exothermic and it is necessary to add a heat exchanger to keep its temperature below 315 K. A heat exchanger with UA = 3000 J/s · K is used. The coolant enters at a mass flow rate of 100 kg/s and a temperature of 285 K.

1. Are the heat exchanger and coolant flow rate adequate to keep the reactor temperature below 315 K?
2. Plot the reactor temperature, T, and the concentrations, C_A, C_B, and C_C as a function of time.

Here are some additional data:

$$k = 0.39175 \cdot \exp\left(5472.7 \cdot \left(\frac{1}{273} - \frac{1}{T}\right)\right)$$

$$K_c = 10^{\frac{3885.44}{T}}$$

ΔH_R° = -79076 J/mol

c_{p_A} = 170.7 J/mol/K

$c_{p_B} = c_{p_C} = c_{p_D} \sim c_{p_{water}} = 75.246$ J/mol/K