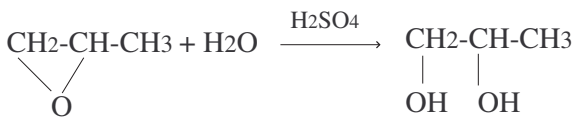
ECH 4323: Chemical Process Control
FINAL PROJECT

Propylene glycol is produced by the hydrolysis of propylene oxide in a CSTR. The reaction is normally conducted using excess water. To get propylene glycol of the desired final specification, the reaction products are sent through a dewatering distillation column.



$$A \quad + \quad B \quad \longrightarrow \quad C$$

The objective of this project is to analyze the steady-state and dynamic behavior of the propylene glycol process and design suitable controllers for the reactor as well as the distillation column.

The following data is available for the reactor part of the process:

1. Reactor volume: 1 m^3
2. Feed Characteristics:
   - Propylene oxide: C_{A0} $kmol/hr$
   - Methanol: 33 $kmol/hr$
   - Water (with 0.1 wt. % H_2SO_4): 365 $kmol/hr$
   - Feed Temperature: T_0 ^oC
3. The reaction is first order with respect to propylene oxide

$$-r_A = kC_A$$

where

$$\begin{aligned} k &= Aexp\left(-\frac{E}{RT}\right) \\ A &= 16.96 \times 10^{12} hr^{-1} \\ E &= 75,200\ kJ/kmol \end{aligned}$$

The heat of reaction as a function of temperature is given by

$$\Delta H_{rxn} = -84,500 - 29.24(T - 293)\ kJ/kmol\ propylene\ oxide$$

where T is the reactor temperature in K.

4. The temperature cannot exceed 52^oC to prevent excessive loss of propylene oxide due to evaporation. For this reason, there is a cooling jacket (with water as the coolant) around the reactor with the following characteristics:

   (a) Coolant inlet temperature: 15^oC

   (b) Coolant flow rate: $\dot{m}_{co}$

   (c) (Overall Heat transfer coeff.)(Area): $UA = 3000\ kJ/kgmol/K$

Additional data on reactants and products:

Density:

Propylene Oxide	14.95 $kmol/m^3$
Methanol	24.71 $kgmol/m^3$
Water	55.37 $kgmol/m^3$

Specific Heat:

Propylene Oxide	146 $kJ/kmol/K$
Methanol	81 $kJ/kmol/K$
Water	75 $kJ/kmol/K$
Propylene Glycol	192 $kJ/kmol/K$

For Report 1, do the following:

1. Compute the steady state values of propylene oxide, propylene glycol, and the reactor temperature for the following conditions:

Coolant flow, $\dot{m}_{co}$ $kmol/hr$	Feed Temp., T_0 ^oC	P.O. in Feed, C_{A0} $kmol/hr$
450	24	20
450	20	20
450	28	20
400	24	20
500	24	20
450	24	16
450	24	24

2. Suppose at time $t = 0$, the reactor is at the same conditions as the feed characteristics of the first line of the above table. Develop a dynamic model for the reactor system. Solve for the time profiles of propylene oxide, propylene glycol and the reactor temperature as a function of time.

3. Suppose the inlet temperature undergoes the following pulse change:

$$T_0 = \begin{cases} 24 & 0 \leq t < 2.5\ hr \\ 28 & 2.5 \leq t < 3\ hr \\ 24 & t \geq 3\ hr \end{cases} \tag{1}$$

   How do the reactor temperature and the concentrations of propylene oxide and propylene glycol change with time?