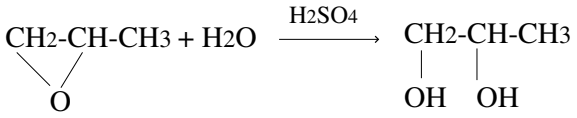
ECH 4323: Chemical Process Control
SIMULATION PROJECT

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.



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: F_{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

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

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 $kJ/kmol/K$

1. Compute the steady state values of propylene oxide, propylene glycol, and the reactor temperature for the following conditions (you may use MATLAB or hand calculations for this part):

Coolant flow, $\dot{m}_{co}$ $kmol/hr$	Feed Temp., T_0 ^oC	P.O. in Feed, F_{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 in MATLAB.

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? Show the appropriate plots in MATLAB.

4. Is the CSTR stable under the following *nominal* conditions?

Coolant flow	450 $kmol/hr$
Feed Temperature	24 ^oC
Propylene Oxide in Feed	20 $kmol/hr$

   Perform a linear stability analysis to answer the above question.

5. Design a distillation column in CHEMCAD that takes the reactor outlet under *nominal conditions* and gives a bottoms product that is 99.5% propylene glycol. Show the CHEMCAD simulation results.

6. What happens in the CHEMCAD simulation when the propylene glycol in the feed to the column is increased or decreased by 10%?

7. Suppose the CSTR is operating at a coolant flow rate of 450 $kmol/hr$ and a propylene oxide feed rate of 20 $kmol/hr$. The initial feed temperature is 20 ^oC. Design

a PI controller in MATLAB that keeps the outlet proplyne glycol concentration at 0.50 $kmol/m^3$. Show the plots of the feed temperature versus time and the proplyne glycol concentration in the outlet versus time.

8. Implement the above controller in CHEMCAD.