## Reactor design tutorial sheet

Q1/ Propylene glycol is produced by hydrating propylene oxide using a solution of 0.1 % sulphuric acid in water as a catalyst. The reaction is:

$$\begin{array}{c} CH_2 & --- & CH & -- & CH_3 + H_2O \rightarrow CH_2 -- & CH & -- & CH_3 \\ | & O & | & OH & | & OH \end{array}$$

An equi-volumetric solution of methanol and propylene oxide flows into a CSTR. At the same time, a 0.1% sulfuric acid solution also flows into the CSTR at a rate of 2.5 times the combined flow rate of propylene oxide and methanol. The coolant is chilled water. Size the reactor, determine the heat exchanger type and area, and calculate the mixer power.

Thermodynamic properties are summarized in Table 1.1, and reaction properties are given below. The heat capacity for propylene glycol was estimated using a rule-of-thumb. The rule states that the majority of low-molecular weight, oxygen-containing organic liquids have a heat capacity of 0.6 cal/g.°F $\pm$ 15% (35 Btu/lbmol.°F). Solve the problem by choosing fill the standard reactor up to the calculated reactor only.

Methanol volumetric flow rate	800 ft <sup>3</sup> /h (22.7 m <sup>3</sup> /h)
Propylene oxide volumetric flow rate	800 ft <sup>3</sup> /h (22.7 m <sup>3</sup> /h)
Acid solution volumetric flow rate	4000 ft <sup>3</sup> /h (113 m <sup>3</sup> /h)
Feed inlet temperature	75°F (23.9°C)
Reaction temperature	100°F (37.8°C)
Chilled water inlet temperature	41°F (5°C)
Chilled water exit temperature	59°F (15°C)
Required propylene oxide conversion	0.37

Data

### **Reaction Properties**

Rate constant at 25°C (77°F)	1.078 h <sup>-1</sup>
Activation energy, E	32,400 Btu/lbmol (75,330 kJ/kgmol)

Component	Molecular Weight	Density <sup>a</sup> g/cm <sup>3</sup>	Heat Capacity <sup>b</sup> Btu/lbmol.°F	Standard Enthalpy of Reaction <sub>c,d</sub> Btu/lbmol
Propylene Oxide	58.08	0.859	35	-66,600
Water	18.02	0.9941	18	-123,000
Propylene Glycol	76.11	1.036	46	-226,000
Methanol	32.04	0.7914	19.5	-

### **Table Thermodynamic Properties for Proplyene Glycol Synthesis**

a) To convert g/cm to kg/m, multiply by 1000.

b) To convert Btu/lbmol.°F to kJ/kgmol.°K, multiply by 4.187.

c) At 25°C (77°F)

d) To convert Btu/lbmol to kJ/kgmol, multiply by 2.325.

# Q2/ For the same problem above, resize the reactor keeping the same conversion inside a standard reactor.

Q3/ In 1973, because of a natural gas shortage, the US evaluated two methods of transporting natural gas from overseas producers. One of these methods was to convert the natural gas to methanol. Then, the methanol would be shipped to the US and converted back to methane in two catalytic reactors in series. The first reactor converts methanol to a mixture of gases, which contains methane. The composition of the gases leaving this reactor, which is given in Table 3.1, becomes the input to the second reactor. In the second reactor, some of the carbon monoxide and dioxide in the mixture is converted to additional methane. Table 3.1 gives the gas analysis out of the second reactor. After the second reactor, the methane is separated from the mixture before entering the natural-gas pipeline. Estimate the reactor size using the space velocity given below.

### Data

Catalyst	nickel deposited on kieselguhr		
Catalyst size	1/8 in tablets (3.18 mm)		
Bed void fraction 0.38	Bed void fraction 0.4		
Bulk density	901b/ft <sup>3</sup> (1440 kg/m <sup>3</sup> )		
Space velocity	3000 h <sup>-1</sup> (at 60°F, 1 atm) (289 K, 1.01 bar)		
Molecular weight in	20.4		
Viscosity of natural gas	0.0195*10 <sup>-3</sup> kg/m.s		

Flow rate in	15433.37 lbmol/h (7000 kgmol/h)
Superficial velocity	1 ft/s (0.3048 m/s)

# **Table Reactor Composition**

Component	Molecular Weight	<b>Reactor Composition Mole Fraction</b>	
		Input	Output
H <sub>2</sub> O	18.02	0.2861	0.30877
CH <sub>4</sub>	16.04	0.4558	0.48139
H <sub>2</sub>	2.0	0.0771	0.03730
СО	28.01	0.1140	0.00015
CO <sub>2</sub>	44.0	0.1696	0.17253
Temperature, K		527.6	588.7
Pressure, bar		27.92	