## 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:


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 $0.6 \mathrm{cal} / \mathrm{g} .{ }^{\circ} \mathrm{F} \pm 15 \%$ ( $35 \mathrm{Btu} / \mathrm{lbmol} .^{\circ} \mathrm{F}$ ). Solve the problem by choosing fill the standard reactor up to the calculated reactor only.

## Data

| Methanol volumetric flow rate | $800 \mathrm{ft}^{3} / \mathrm{h}\left(22.7 \mathrm{~m}^{3} / \mathrm{h}\right)$ |
| :---: | :---: |
| Propylene oxide volumetric flow rate | $800 \mathrm{ft}^{3} / \mathrm{h}\left(22.7 \mathrm{~m}^{3} / \mathrm{h}\right)$ |
| Acid solution volumetric flow rate | $4000 \mathrm{ft}^{3} / \mathrm{h}\left(113 \mathrm{~m}^{3} / \mathrm{h}\right)$ |
| Feed inlet temperature | $75^{\circ} \mathrm{F}\left(23.9^{\circ} \mathrm{C}\right)$ |
| Reaction temperature | $100^{\circ} \mathrm{F}\left(37.8^{\circ} \mathrm{C}\right)$ |
| Chilled water inlet temperature | $41^{\circ} \mathrm{F}\left(5^{\circ} \mathrm{C}\right)$ |
| Chilled water exit temperature | $59^{\circ} \mathrm{F}\left(15^{\circ} \mathrm{C}\right)$ |
| Required propylene oxide conversion | 0.37 |

## Reaction Properties

| Rate constant at $25^{\circ} \mathrm{C}\left(77^{\circ} \mathrm{F}\right)$ | $1.078 \mathrm{~h}^{-1}$ |
| :---: | :---: |
| Activation energy, E | $32,400 \mathrm{Btu} / \mathrm{lbmol}(75,330 \mathrm{~kJ} / \mathrm{kgmol})$ |

Table Thermodynamic Properties for Proplyene Glycol Synthesis

| Component | Molecular Weight | $\begin{gathered} \text { Density }^{\mathrm{a}} \\ \mathrm{~g} / \mathrm{cm}^{3} \end{gathered}$ | Heat Capacity ${ }^{b}$ Btu/lbmol. ${ }^{\circ}{ }^{\circ}$ | Standard Enthalpy of Reaction 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 | - |

a) To convert $\mathrm{g} / \mathrm{cm}$ to $\mathrm{kg} / \mathrm{m}$, multiply by 1000 .
b) To convert $\mathrm{Btu} / \mathrm{lbmol} .{ }^{\circ} \mathrm{F}$ to $\mathrm{kJ} / \mathrm{kgmol} .{ }^{\circ} \mathrm{K}$, multiply by 4.187 .
c) At $25^{\circ} \mathrm{C}\left(77^{\circ} \mathrm{F}\right)$
d) To convert Btu/lbmol to $\mathrm{kJ} / \mathrm{kgmol}$, 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 $(3.18 \mathrm{~mm})$ |
| Bed void fraction 0.38 | Bed void fraction 0.4 |
| Bulk density | $901 \mathrm{~b} / \mathrm{ft}^{3}\left(1440 \mathrm{~kg} / \mathrm{m}^{3}\right)$ |
| Space velocity | $3000 \mathrm{~h}^{-1}\left(\mathrm{at} 60^{\circ} \mathrm{F}, 1 \mathrm{~atm}\right)(289 \mathrm{~K}, 1.01 \mathrm{bar})$ |
| Molecular weight in | 20.4 |
| Viscosity of natural gas | $0.0195^{*} 10^{-3} \mathrm{~kg} / \mathrm{m} . \mathrm{s}$ |


| Flow rate in | $15433.37 \mathrm{lbmol} / \mathrm{h}(7000 \mathrm{kgmol} / \mathrm{h})$ |
| :---: | :---: |
| Superficial velocity | $1 \mathrm{ft} / \mathrm{s}(0.3048 \mathrm{~m} / \mathrm{s})$ |

Table Reactor Composition

| Component | Molecular Weight | Reactor Composition Mole Fraction |  |
| :---: | :---: | :---: | :---: |
|  |  | Input | Output |
| $\mathrm{H}_{2} \mathrm{O}$ | 18.02 | 0.2861 | 0.30877 |
| $\mathrm{CH}_{4}$ | 16.04 | 0.4558 | 0.48139 |
| $\mathrm{H}_{2}$ | 2.0 | 0.0771 | 0.03730 |
| CO | 28.01 | 0.1140 | 0.00015 |
| $\mathrm{CO}_{2}$ | 44.0 | 0.1696 | 0.17253 |
| Temperature, K |  | 527.6 | 588.7 |
| Pressure, bar |  | 27.92 |  |

