CL-402: Chemical Process Technology

July-November session, 2018

7th semester, Department of Chemical Engineering Indian Institute of Technology Guwahati, Guwahati

Tutorial 2

Use Aspen Plus V8.8 to solve all the problems.

Problem-1: Ammonia Production

Nitrogen and hydrogen react to form ammonia in the presence of a catalyst,

 $\frac{1}{2}N_2 + \frac{3}{2}H_2 \Longrightarrow NH_3$

The reactor in which this reaction is to be run is maintained at 450 K.

a. What will be the mole fractions of nitrogen, hydrogen, and ammonia exiting the reactor if stoichiometric amounts of nitrogen and hydrogen enter the reactor, which is kept at 4 bar?
b. What will be the exit mole fractions if the reactor operates at 4 bar and the feed consists of 0.5 kmol/hr of nitrogen, 1.5 kmol/hr of hydrogen and 2.0 kmol/hr argon?

c. For a feed consisting of stoichiometric amounts of nitrogen and hydrogen, study the effect of reaction temperature on ammonia production in the range 200-700 °C and also the effect of reaction pressure on ammonia production in the range of 100-1000 bar.

Problem-2: Isomerization of Normal Butane

Normal butane, C_4H_{10} , is to be isomerized to isobutane in a plug-flow reactor. This elementary reversible reaction is to be carried out adiabatically in the liquid phase under high pressure using a liquid catalyst. The feed enters at 330 K.

Isomerization reaction:

$$n-C_4H_{10} \Longrightarrow i-C_4H_{10}$$

Both forward and reverse reactions are 1st order with respect to reactants.

$$Rate_{forward} = k_f C_{C4H10}$$
, and $Rate_{reverse} = k_b C_{iC4H10}$

where,

$$k_f = 0.008639 * Exp\left[\frac{65700000}{R}\left(\frac{1}{360} - \frac{1}{T}\right)\right]$$
 and, $k_b = 0.003442 * Exp\left[\frac{72600000}{R}\left(\frac{1}{360} - \frac{1}{T}\right)\right]$

where, k_f and k_b are in sec^{-1} , Temperature in K,reactant concentration in terms of molarity (kmol/ m^3) and activation energy in J/kmol.

 Calculate the PFR volume for 70% conversion(feed rate = 160 kmol/h, 90 mol% n-butane and 10 mol% of i-pentane(which is considered an inert)).

2. Plot the molar composition of all the components along the length of the reactor. Also plot the temperature profile along the length of the reactor.

3. Calculate the CSTR volume for the same conditions as the PFR.

Problem 1



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Sensitivity Analysis

To study the effect of temp. and press. on ammonia yield



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Effect of Temp. and Pressure on NH₃ yield.



Problem 2









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Repeat the above steps for CSTR.







To find the CSTR reactor volume for 70% conversion, we will use "**Design Specs**" feature of Aspen Plus.

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Reactor	Volume (m ³)
PFR	3.14
CSTR	20.7

For 70% conversion, CSTR volume is approx. 6.6 times PFR.

THE END