CE 329 Fall 2015

Class 20 Worksheet

A gas mixture contains 1500 ppm of A, 1000 ppm of B and 7% C. The remainder of the gas is inert (non-reactive). A 3 L reactor steel reactor is charged with this mixture at 1115 K and 1.7 atm. Reactions (1) and (2) take place adiabatically with rates given by equations (3) and (4). The pre-exponential factors for reactions (1) and (2) are 6.1 x 10^{16} L mol^{-1} s^{-1} and 5.5 x 10^{13} s^{-1}, respectively, and the activation energies are 250 and 320 kJ/mol, respectively. Calculate the parts per million of B after 0.5, 1 and 5 seconds. You may assume the heats of reactions (1) and (2) to be constant and equal to -1700 kJ/mol and -800 kJ/mol, respectively. The heat capacities of the gases may be taken to equal that of the inert, 32 J mol^{-1} K^{-1}, and to be independent of temperature.

$$4\ A + 4\ B + C \rightarrow 4\ Y + 6\ Z \tag{1}$$

$$4\ A + 5\ C \rightarrow 4\ B + 6\ Z \tag{2}$$

$$r_1 = k_{0,1} \exp\left\{\frac{-E_1}{RT}\right\} C_A C_B \tag{3}$$

$$r_2 = k_{0,2} \exp\left\{\frac{-E_2}{RT}\right\} C_A \tag{4}$$

Read through the problem statement and determine the type of reactor being used, whether it operates transiently or at steady state, whether it is heated/cooled, isothermal or adiabatic and (if the reactor is a PFR) whether there is a significant pressure drop

Read through the problem statement a second time. Assign each quantity given in the problem statement to the appropriate variable symbol. If all of the given quantities are intensive, select a value for one extensive variable as the basis for your calculations. Determine what quantities the problem asks for and assign appropriate variable symbols to them

Write a mole balance equation for each reactant and product; expand all summations and continuous products, and eliminate all zero-valued and negligible terms

Write an energy balance design equation (unless the reactor is isothermal and the problem does not ask any questions related to heat transfer); expand all summations and continuous products, and eliminate all zero-valued and negligible terms. If information about the heat transfer fluid, beyond its temperature, is provided, write an energy balance on the heat transfer fluid

If the reactor is a PFR and there is a significant pressure drop, write a momentum balance; expand all summations and continuous products, and eliminate all zero-valued and negligible terms

Identify the type of the design equations

- if they are algebraic, identify the unknowns
  - the number of unknowns must equal the number of equations
- if they are differential, identify the independent and dependent variables
  - if the number of dependent variables is greater than the number of equations, choose one dependent variable and express it and its derivatives in terms of the remaining dependent variables

Determine what you will need to provide in order to solve the design equations numerically and show how to do so

After the design equations have been solved numerically, yielding values for the unknowns (algebraic equations) or the independent and dependent variables (differential equations), use the results to calculate any other quantities or plots that the problem asked for