A First Course on Kinetics and Reaction Engineering

Activity 1.1

Problem Purpose

This problem will allow you to practice using stoichiometry to generate expressions for quantities related to the progress of a reaction.

Problem Statement

Consider the reaction 4 NH_3 + 5 O_2 → 4 NO + 6 H_2O taking place in a closed, constant volume reactor (V = 1 L). At the start of the process, the reactor held one mole of NH_3 and 0.15 mole of O_2.

1. To solve some problems in this course, you will need to write an expression for the concentration of O_2 in terms of the concentration of NH_3 and the initial composition of the system.
2. To solve other problems (in Part I of the course) you will need to write expressions for the mole fractions of each of the four species (NH_3, O_2, NO and H_2O) in terms of the extent of the reaction and the initial composition of the system.
3. To solve still other problems in CE 329, you will need to calculate the concentration of O_2, given the fractional conversion of NH_3 and the initial composition of the system.

You will work as a group of 3 students to solve one of these three problems. Each group member should fill out this worksheet as you solve the problem assigned to you because once you are done you will be re-grouped with two students who solved the other problems and will be expected to explain how your problem was solved.

Worksheet

1. Generate a mole table for this problem

2. Go through the problem statement, and
    a. assign each quantity that is given to the corresponding variable
    b. assign a variable to each quantity you have been asked to calculate

3. Examine all of the quantities given in the problem statement; if no extensive variables are specified, choose one and assume a value for it as your calculation basis.

4. For every variable listed in step 2 that is defined in terms of the moles (for a batch system) or the molar flow rates (for a flow system)
    a. write the defining equation and
    b. if the definition includes additional unknown quantities, add those variables to the list from step 2b
        i. if these quantities can be written in terms of the moles or molar flow rates, write the corresponding equations

5. In the set of equations from step 4, each time moles or molar flow rate appears, express it in terms of the extent(s) of the independent reactions. This should yield a set of N equations in N unknowns. If so, solve them and use the result to calculate what you were asked to find; if not, look for additional relationships between the variables.

6. Use this page to outline the solution to the problems you did not solve as your re-grouped group members explain them to you.