A First Course on Kinetics and Reaction Engineering

Unit 1. Activity 1 Solution

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.

Solution

Analysis: In these problems you know the starting composition of the system and the stoichiometry of the reaction. You are given some information related to how much reaction has taken place and asked to calculate values or expressions for other quantities when that much reaction has taken place. The problem statement doesn't give enough information to use reactor models, and it doesn't mention thermodynamic equilibrium, so it must be possible to obtain the answers just from the stoichiometry, the initial composition and the reaction progress variable you have been given.

Approach: A mole table offers a concise way to summarize the information you are given and to derive the expressions you will need. Once the mole table is set up, you can use it to express the reaction progress variable that you know in terms of the extent of reaction and to express the desired quantity in terms of the extent of reaction. Solving one of the resulting expressions for the extent of reaction and substituting into the other expression will lead to the desired answer.

Execution: A mole table for this problem is given as Table 1. When generating a mole table, the two most important things to remember are to use a mathematically independent set of reactions and to use the proper signs with the stoichiometric coefficients (reactants are negative). Here there is only one reaction, so it must be mathematically independent.

Table 1. Mole Table for Activity 1.

Species	***Initial Moles***	***Final Moles***
NH_3	1	$1-4\xi$
O_2	0.15	$0.15-5\xi$
NO	0	4ξ
H_2O	0	6ξ
Total	1.15	$1.15+\xi$

1. For this question, we are given the concentration of NH_3, and asked to generate an expression for the concentration of O_2. By definition, concentrations are equal to the number of moles divided by the volume. By use of the mole table, these can each be expressed in terms of the extent of the reaction, as shown in equations (1) and (2), where the final units will be mol L^{-1}.

$$C_{NH_3} = \frac{n_{NH_3}}{V} = \frac{1-4\xi}{1} = 1-4\xi \tag{1}$$

$$C_{O_2} = \frac{n_{O_2}}{V} = \frac{0.15-5\xi}{1} = 0.15-5\xi \tag{2}$$

Solving equation (1) for the extent of reaction gives equation (3). Substitution of equation (3) into equation (2) and simplification gives the desired answer, equation (4).

$$\xi = \frac{1-C_{NH_3}}{4} \tag{3}$$

$$C_{O_2} = 0.15 - 5\left(\frac{1-C_{NH_3}}{4}\right) = 0.15 - 1.25 + 1.25C_{NH_3}$$

$$C_{O_2} = 1.25C_{NH_3} - 1.1 \tag{4}$$

2. For this question, we are asked for expressions for the mole fractions in terms of the extent of reaction. By definition, the mole fraction of a species is the number of moles of that species divided by the total number of moles. We can then obtain the desired expressions directly by substitution from the mole table, as shown in equations (5) through (8).

$$y_{NH_3} = \frac{n_{NH_3}}{n_{total}} = \frac{1-4\xi}{1.15+\xi} \tag{5}$$

$$y_{O_2} = \frac{n_{O_2}}{n_{total}} = \frac{0.15 - 5\xi}{1.15 + \xi} \tag{6}$$

$$y_{NO} = \frac{n_{NO}}{n_{total}} = \frac{4\xi}{1.15 + \xi} \tag{7}$$

$$y_{H_2O} = \frac{n_{H_2O}}{n_{total}} = \frac{6\xi}{1.15 + \xi} \tag{8}$$

3. For this question we are given the fractional conversion of NH_3, and we are asked to calculate the concentration of O_2. Equation (9) is the defining equation for the fractional conversion, where by substitution from the mole table it has been expressed in terms of the extent of reaction.

$$f_{NH_3} = \frac{n_{NH_3}^0 - n_{NH_3}}{n_{NH_3}^0} = \frac{1 - (1 - 4\xi)}{1} = 4\xi \tag{9}$$

We already have expressed the concentration of O_2 in terms of the extent of reaction in equation (2). Equation (9) can be solved for the extent of reaction, equation (10), and the result can be substituted into equation (2). This gives the desired answer, equation (11), for calculating the concentration of O_2 from the fractional conversion of NH_3.

$$\xi = \frac{f_{NH_3}}{4} \tag{10}$$

$$C_{O_2} = 0.15 - 5\left(\frac{f_{NH_3}}{4}\right) = 0.15 - 1.25 f_{NH_3} \tag{11}$$