REB, The Course
Class 2, Activity 1 Solution

The gas phase reaction synthesis of ammonia from NO, reaction (1), takes place in a system that initially contained 2 moles of H_2 and 1 mole of NO. If 50% of the limiting reactant was converted, what was the final mole fraction of ammonia?

$$2NO + 5H_2 \rightarrow 2NH_3 + 2H_2O \tag{1}$$

Identify the limiting reactant by calculating the thermodynamic equivalences of NO and H_2.

$$\frac{n_{NO,0}}{|\nu_{NO}|} = \frac{1 \text{ mol}}{|-2|} = 0.5 \text{ mol} \tag{1}$$

$$\frac{n_{H_2,0}}{|\nu_{H_2}|} = \frac{2 \text{ mol}}{|-5|} = 0.4 \text{ mol} \tag{2}$$

The stoichiometric equivalence of H_2 is smaller that that of NO, so H_2 is the limiting reactant. Now use the given information (initial molar amounts and conversion) to calculate the apparent extent of reaction.

$$f_{H_2} = \frac{n_{H_2,0} - n_{H_2}}{n_{H_2,0}} = \frac{n_{H_2,0} - \left(n_{H_2,0} - 5\xi\right)}{n_{H_2,0}} = \frac{5\xi}{n_{H_2,0}}$$

$$\frac{f_{H_2} n_{H_2,0}}{5} = \xi = \frac{0.5\,(2 \text{ mol})}{5} = 0.2 \text{ mol} \tag{3}$$

Then use the apparent extent to calculate the quantity of interest (mole fraction of ammonia).

$$n_{NO} = n_{NO,0} - 2\xi = 1 \text{ mol} - 2\,(0.2 \text{ mol}) = 0.6 \text{ mol}$$

$$n_{H_2} = n_{H_2,0} - 5\xi = 2 \text{ mol} - 5\,(0.2 \text{ mol}) = 1.0 \text{ mol}$$

$$n_{NH_3} = n_{NH_3,0} + 2\xi = 0 \text{ mol} + 2\,(0.2 \text{ mol}) = 0.4 \text{ mol}$$

$$n_{H_2O} = n_{H_2O,0} + 2\xi = 0 \text{ mol} + 2\,(0.2 \text{ mol}) = 0.4 \text{ mol}$$

$$n_{total} = n_{NO} + n_{H_2} + n_{NH_3} + n_{H_2O} = \left(0.6 + 1.0 + 0.4 + 0.4\right) \text{ mol} = 2.4 \text{ mol}$$

$$y_{NH_3} = \frac{n_{NH_3}}{n_{total}} = \frac{0.4}{2.4} = 0.167$$