REB, The Book
Example 2.6.3 Solution

Suppose gas-phase reaction (1) was studied in an open, steady-state, isothermal, isobaric system. The flow into the system contained 0.5 mol min^{-1} of N_2O_5 and 0.5 mol min^{-1} of N_2 at 600 K and 5 MPa.

(a) Write an equation for the outlet molar flow rate of NO_2 in terms of the outlet molar flow rate of N_2O_5.
(b) If the outlet flow contains 30% N_2, calculate the conversion of N_2O_5.

$$2\ N_2O_5 \rightleftarrows 4\ NO_2 + O_2 \tag{1}$$

(a) An expression for the apparent extent of reaction can be written in terms of the change in the amount of N_2O_5, equation (2), and in terms of the change in the amount of NO_2, equation (3). The extent must be the same in both cases, so setting the expressions equal to each other and rearranging yields the requested expression for the outlet molar flow rate of NO_2 in terms of the outlet molar flow rate of N_2O_5, equation (4).

$$\dot{n}_{N_2O_5} = \dot{n}_{N_2O_5,in} - 2\dot{\xi} \quad \Rightarrow \quad \dot{\xi} = \frac{\dot{n}_{N_2O_5,in} - \dot{n}_{N_2O_5}}{2} \tag{2}$$

$$\dot{n}_{NO_2} = \cancel{\dot{n}_{NO_2,in}} + 4\dot{\xi} \quad \Rightarrow \quad \dot{\xi} = \frac{\dot{n}_{NO_2}}{4} \tag{3}$$

$$\frac{\dot{n}_{N_2O_5,in} - \dot{n}_{N_2O_5}}{2} = \frac{\dot{n}_{NO_2}}{4} \quad \Rightarrow \quad \dot{n}_{NO_2} = 2\left(\dot{n}_{N_2O_5,in} - \dot{n}_{N_2O_5}\right) \tag{4}$$

(b) Noting that the inlet molar flow rates of NO_2 and O_2 are zero, expressions for the outlet molar flow rates of the reagents are given in equations (5) through (8), and by adding them an expression for the total outlet molar flow rate, equation (9), is obtained.

$$\dot{n}_{N_2O_5} = \dot{n}_{N_2O_5,in} - 2\dot{\xi} \tag{5}$$

$$\dot{n}_{NO_2} = 4\dot{\xi} \tag{6}$$

$$\dot{n}_{O_2} = \dot{\xi} \tag{7}$$

$$\dot{n}_{N_2} = \dot{n}_{N_2,in} \tag{8}$$

$$\dot{n}_{total} = \dot{n}_{total,in} + 3\dot{\xi} \tag{9}$$

The outlet mole fraction of N_2 can be expressed in terms of the apparent extent of reaction as shown in equation (10). The apparent extent of reaction found by solving that equation can be used to calculate the outlet molar flow rate of N_2O_5 according to equation (5), after which the conversion can be found using equation (11).

$$y_{N_2,out} = \frac{\dot{n}_{N_2}}{\dot{n}_{total}} = \frac{\dot{n}_{N_2,in}}{\dot{n}_{total,in} + 3\dot{\xi}} \tag{10}$$

$$f_{N_2O_5} = \frac{\dot{n}_{N_2O_5,in} - \dot{n}_{N_2O_5}}{\dot{n}_{N_2O_5,in}} \tag{11}$$

The calculations were performed as described above. The apparent extent of reaction is 0.222 mol min^{-1}, the outlet molar flow rate of N_2O_5 is 0.056 mol min^{-1}, and the conversion is 88.9%.