Name: ____________________

Date: _____________

PROBLEM 5.38

Propylene is hydrogenated in a batch reactor:

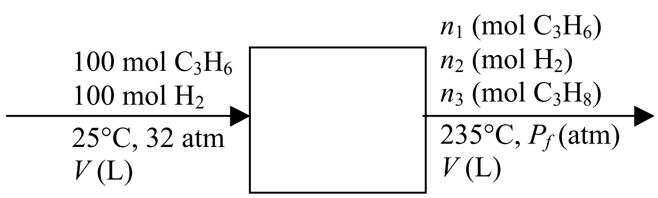
$$C_3H_6(g) + H_2(g) \longrightarrow C_3H_8(g)$$

Equimolar amounts of propylene and hydrogen are fed into the reactor at 25°C and a total absolute pressure of 32.0 atm, and some time later the temperature is 235°C. You may assume ideal gas behavior for this problem, although at the high pressures involved this assumption constitutes a crude approximation at best.

(a) If the reaction goes to completion at 235°C, what would be the final pressure?
(b) If the pressure is 35.1 atm and the temperature is 235°C, what percentage of the propylene fed has reacted?
(c) Construct a graph of pressure versus fractional conversion of propylene, assuming T = 235°C. Use a graph to confirm the results in parts (a) and (b). (Note: We'll use E-Z Solve for this part.)

Strategy

Since we are not told how much of the reaction mixture is charged, we'll choose a basis of 100 mol C_3H_6, and since the feed is equimolar in propylene and hydrogen there must also be 100 mol H_2. We know the extent of reaction but not the pressure in part (a) and vice versa in part (b), so we label the chart as though neither is known. Also, we assume that the reaction volume is the same throughout the reaction. (Put another way, we assume the reactor is a rigid vessel and not an expandable balloon or a cylinder with a movable piston.)



(a) If the reaction goes to completion at 235°C, what would be the final pressure?

Solution

If the reaction is complete, we can easily determine the three unknown molar quantities in the outlet stream labeling. (*Hint*: Use the expression for n_1 to find the extent and then use the extent to find n_2 and n_3).

$$n_1 = 0 \text{ mol } C_3H_6,\ \ n_2 = \underline{\qquad} \text{ mol } H_2,\ \ n_3 = \underline{\qquad} \text{ mol } C_3H_8 \tag{5.38-1}$$

We are left with two unknowns (V and P_f), and we can write two equations to determine them (the ideal gas equation-of-state at the inlet and outlet). Since we are not interested in V, the most efficient solution method is to eliminate it between the two equations and solve for the final pressure.

$$\begin{array}{l}\textbf{Initial: } (32 \text{ atm})V = (200 \text{ mol})R(298\text{K}) \\ \textbf{Final: } P_f V = (100 \text{ mol})R(508\text{K})\end{array} \xrightarrow[\text{by } 1^{st}]{\text{Divide } 2^{nd}} \frac{P_f}{32 \text{ atm}} = \frac{\underline{\qquad}}{\underline{\qquad}} \Rightarrow P_f = \underline{\qquad} \text{ atm} \tag{5.38-2}$$