Determine the theoretical yield for the combustion of octane if 1 liter of octane fuel is mixed with 1420 liters of O_2. Please first balance the chemical equation. [The density of octane is 0.7 gm/cm^3]

$$C_8H_{18}(\ell) + \ O_2(g) \rightarrow \ CO_2(g) + \ H_2O\ (\ell)$$

Solution: Step 1. Balance the chemical equation:

$$C_8H_{18}(\ell) + \frac{25}{2} O_2(g) \rightarrow 8\, CO_2(g) + 9 H_2O\ (\ell)$$

Step 2. calculate the number of moles of C_8H_{18} and O_2 as reactants.

$$n_1 = \frac{\rho_1 V_1}{M_{m,1}} = \frac{(0.70)(1)(1000)}{114} = 6.14\, mol$$

The factor of 1000 converts from cm^3 to L.

Determine the theoretical yield for the combustion of octane if 1 liter of octane fuel is mixed with 1420 liters of O_2.

$$C_8H_{18}(\ell) + \frac{25}{2}O_2(g) \rightarrow 8\,CO_2(g) + 9H_2O\ (\ell)$$

Step 2 (contd.). Let's conduct a unit analysis of the expression we used on the previous slide.

$$n_1 = \frac{\rho_1 \mathrm{V}_1}{\mathrm{M}_{\mathrm{m},1}} = \frac{(\mathrm{gm}/cm^3)(\mathrm{L})(cm^3/L)}{\mathrm{gm/mol}} = mol$$

And of course the molar mass of octane is

$$M_m = 8(12) + 18 = 114\ amu$$

Determine the theoretical yield for the combustion of octane if 1 liter of octane fuel is mixed with 1420 liters of O_2.

$$C_8H_{18}(\ell) + \frac{25}{2}O_2(g) \rightarrow 8\,CO_2(g) + 9H_2O\ (\ell)$$

Step 2 (contd.). calculate the number of moles of C_8H_{18} and O_2 as reactants.

$$n_1 = \frac{\rho_1 V_1}{M_{m,1}} = \frac{(0.70)(1)(1000)}{114} = 6.14\,mol$$

$$n_2 = \frac{PV_2}{RT} = \frac{(1\,atm)(1420\,L)}{\left(0.08206\,\frac{Latm}{molK}\right)(298\,K)} = 58.1\,moles$$

Determine the theoretical yield for the combustion of octane if 1 liter of octane fuel is mixed with 1420 liters of O_2.

$$C_8H_{18}(\ell) + \frac{25}{2}O_2(g) \rightarrow 8\,CO_2(g) + 9H_2O\;(\ell)$$

Step 3. Compare the actual molar ratio to the stoichiometry

$$Actual = \frac{n_2}{\mathrm{n}_1} = \frac{58.1}{6.14} = 9.46$$

The stoichiometry requires a ratio of 12.5. We will run out of O_2 before the combustion is complete. The ratio of the actual to theoretically required O_2 is

$$Yield = \frac{9.46}{12.5} = 0.756 = 75.6\%$$