Homework #2 Due: Sept. 10
Name ________________________ Chemistry 331

Consider a cylinder in a 4 liter V-8 engine (i.e. 8 cylinders with a total expanded volume of 4 liters). Let's look at the work extracted during expansion in two phases:

I. Isothermal expansion
II. Adiabatic cooling and expansion

1. Calculate the maximum isothermal work of expansion possible when 0.05 moles of n-octane is combusted perfectly in a cylinder at a temperature of 500 K. Assume that H_2O in the combusted products is a gas. Assume that the initial headspace volume during fuel injection is 0.002 L. Assume further that the isothermal expansion is carried out only to 0.142 L.

Solution: According to the chemical reaction for combustion, for each of mole of octane combusted 17 moles of gas are produced.

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

Thus, there are 0.85 moles of gas.
$w = -nRT\ln(V_2/V_1) = -(0.85\ \text{mol})(8.31\ \text{J/mol-K})(500\ \text{K})\ln(0.142/0.002) = -15\ \text{kJ}$

2. The ambient temperature is 300 K. Assuming that the gas in the cylinder cools adiabatically, how much further would the gas expand. You may assume that the heat capacity for a diatomic gas applies here.

Solution: For an adiabatic expansion of a diatomic ideal gas the following applies

$$V_2 = V_1\left(\frac{T_1}{T_2}\right)^{5/2} \quad \textit{for an ideal diatomic gas}$$

$$V_2 = (0.142\ L)\left(\frac{500}{300}\right)^{5/2} = (0.142)(3.58)\ L = 0.5\ L$$

3. Calculate the work done during the adiabatic expansion.

   Solution: for the adiabatic expansion q = 0 so $w = \Delta U = C_V\Delta T$.
   Therefore, $w = 3\ nR(T_2 - T_1) = 3(0.85\ \text{mol})(8.31\ \text{J/mol-K})(300\ \text{K} - 500\ \text{K})$
   $= -4238\ \text{J}$

4. Imagine that the design for the engine was very poor and that the isothermal step in question 1 was a one step expansion against an external pressure of 1 atm. Calculate the work of expansion in this case (again from 0.002 to 0.142 L).
   Solution: $w = -P_{ext}\Delta V = -(1\ \text{atm})(0.142 - 0.002)\text{L} = 0.14\ \text{L-atm} = -14.18\ \text{J}$

5. Assume that an adiabatic expansion is carried out following the single-step irreversible expansion. Calculate the final volume.

Solution: It is the same as in question 2. Internal energy is a state function.

6. Calculate the work of adiabatic expansion following the single-step irreversible expansion step of question 4.

   Solution: It is the same as in question 3. Internal energy is a state function.