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# Jet and Rocket Propulsion

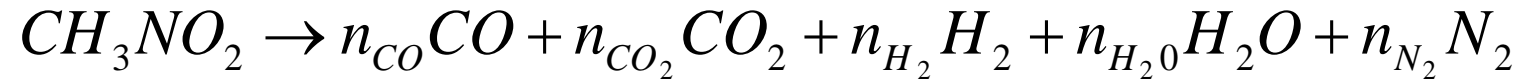
## AE4451

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LECTURE 10 class example

# Example problem

The following reaction describes the decomposition of the liquid monopropellant nitromethane into 5 different gaseous products :



Using the water-gas reaction known to be written:



Determine the following:

(i) the number of moles of each product from the decomposition of nitromethane

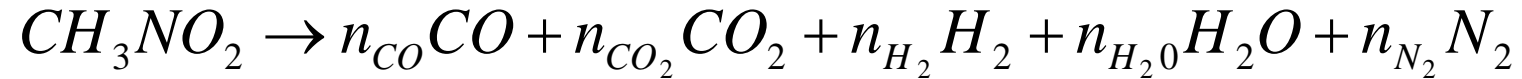
(ii) the combustion temperature

heat of formation  
enthalpy change from reference to imposed T of 2500

species	$\Delta_f H^0$	$\Delta h_j^{2500}$
N <sub>2</sub>	0	74.296
H <sub>2</sub> O	-241.826	99.108
H <sub>2</sub>	0	70.498
CO	-110.53	74.985
CO <sub>2</sub>	-393.522	121.917
CH <sub>3</sub> NO <sub>2</sub>	-113.1	

# Example problem

(1) let's start with the atom balance for this reaction:



where  $n_x$  = number of moles of the subscripted compound  $x$

- for each element, we check the numbers of atoms present on the left hand side (in the reactants), and compare this to the numbers of atoms found on the right hand side (in the products). This gives:

(i) C:  $1 = n_{CO} + n_{CO_2}$

(ii) H:  $3 = 2n_{H_2} + 2n_{H_2O}$

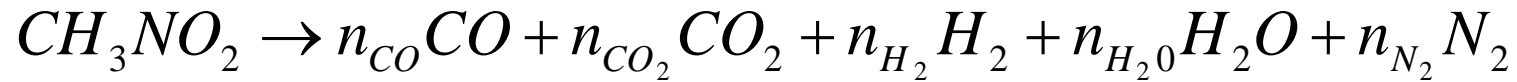
(iii) O:  $2 = n_{CO} + 2n_{CO_2} + n_{H_2O}$

(iv) N:  $1 = 2n_{N_2}$

- since  $N$  appears in only one product on the right hand side, we can see immediately from (iv) that

$$n_{N_2} = 0.5$$

# Example problem



(2) we now have 4 unknown mole ratios, an unknown combustion temperature, and 3 equations. We can use the water-gas reaction given in our problem statement to help.

- recall (**Lecture 8**) that we could write the equilibrium constant  $K_p$  in terms of partial pressures (or simply mole ratios).

e.g. mole ratio of  $CO_2$  in the products is given by 
$$\frac{n_{CO_2}}{n_{CO}CO + n_{CO_2}CO_2 + n_{H_2}H_2 + n_{H_2O}H_2O + n_{N_2}N_2}$$

- for the given water-gas reaction, we can write: 
$$K_p(T) = \frac{n_{H_2O}n_{CO}}{n_{CO_2}n_{H_2}}$$

This gives us a 4th equation. We can in theory solve for the mole ratios, provided we specify a combustion temperature to use, which sets our  $K_p$

# Example problem

summary of our equations so far:

$$(i) \quad 1 = n_{CO} + n_{CO_2}$$

$$(ii) \quad 3 = 2n_{H_2} + 2n_{H_2O}$$

$$(iii) \quad 2 = n_{CO} + 2n_{CO_2} + n_{H_2O}$$

$$(iv) \quad 1 = 2n_{N_2}$$

$$(v) \quad K_p n_{CO_2} n_{H_2} = n_{H_2O} n_{CO}$$

we can choose to solve for any of the unknowns, e.g.  $n_{H_2O}$

$$(iii) - (i) \text{ gives } 1 = n_{CO_2} + n_{H_2O}; \quad n_{CO_2} = 1 - n_{H_2O}$$

$$\text{from (i): } n_{CO} = 1 - n_{CO_2} = n_{H_2O} \quad \text{i.e. same number of moles of CO and H}_2\text{O}$$

$$\text{and from (ii): } n_{H_2} = \frac{3}{2} - n_{H_2O}$$

$$(v) \text{ can be written } K_p n_{CO_2} n_{H_2} = n_{H_2O}^2$$

# Example problem

substituting to leave (v) only in terms of moles of H<sub>2</sub>O:

$$K_p n_{CO_2} n_{H_2} = n_{H_2O}^2$$

$$K_p (1 - n_{H_2O}) \left( \frac{3}{2} - n_{H_2O} \right) = n_{H_2O}^2$$

$$n_{H_2O}^2 \left( \frac{1}{K_p} - 1 \right) + 2.5 n_{H_2O} - 1.5 = 0$$

The temperature 2500 K corresponds to a K<sub>p</sub> value of **6.440** for the water-gas reaction (this will be given to you)

substituting our K<sub>p</sub> value and solving the above quadratic equation gives us

$$n_{H_2O} = \cancel{2.123}, 0.836 \quad (\text{obviously, we can only use the root which is } < 1)$$

$$\Rightarrow n_{CO} = 0.836$$

$$\Rightarrow n_{CO_2} = 0.164 \Rightarrow n_{H_2} = 0.664$$

and from our atom balance equations, we had already found that  $n_{N_2} = 0.5$

# Example problem

(3) Now that we have these values, we can verify the validity of the temperature we imposed, by checking that the heat of our reaction (calculated with the moles we determined) matches the enthalpy rise

$$\Delta_r H^0 = \sum (n \Delta_f H^0)_{\text{products}} - \sum (n \Delta_f H^0)_{\text{reactants}}$$

overall heat of reaction      i.e. formation enthalpies x number of moles  $n$

species	$\Delta_f H^0$	$n$
N <sub>2</sub>	0	0.500
H <sub>2</sub> O	-241.826	0.836
H <sub>2</sub>	0	0.664
CO	-110.53	0.836
CO <sub>2</sub>	-393.522	0.164
CH <sub>3</sub> NO <sub>2</sub>	-113.1	1

$$\Delta_r H^0 = \left[ \begin{array}{l} \text{N}_2 \qquad \qquad \text{H}_2\text{O} \\ (0.5 \times 0) + (0.836 \times -241.826) + \\ (0.664 \times 0) + (0.836 \times -110.53) + (0.164 \times -393.522) \\ \text{H}_2 \qquad \qquad \text{CO} \qquad \qquad \text{CO}_2 \end{array} \right] - (1 \times -113.1) \quad \text{CH}_3\text{NO}_2$$

$\Delta_r H^0 = 246 \text{ KJ/mol}$

# Example problem

(4) We can calculate the enthalpy rise using the JANAF tables as well, at the temperature 2500 K

overall enthalpy rise  $\Delta H_{298}^{2500} = \underbrace{\sum n_j \Delta h_j}$

i.e. enthalpy change for our product species going from reference temp 298 K to 2500 K, x number of moles  $n$

species	$\Delta h_j^{2500}$	$n_f$
N <sub>2</sub>	74.296	0.500
H <sub>2</sub> O	99.108	0.836
H <sub>2</sub>	70.498	0.664
CO	74.985	0.836
CO <sub>2</sub>	121.917	0.164
CH <sub>3</sub> NO <sub>2</sub>		1

$$\Delta H_{298}^{2500} = (0.5 \times \overset{\text{N}_2}{74.296}) + (0.836 \times \overset{\text{H}_2\text{O}}{99.108}) + (0.664 \times \underset{\text{H}_2}{70.498}) + (0.836 \times \underset{\text{CO}}{74.985}) + (0.164 \times \underset{\text{CO}_2}{121.917})$$

$\Delta H_{298}^{2500} = 249.49 \text{ KJ/mol}$

# Example problem

Notice how

$$\Delta_r H^0 \neq \Delta H_{298}^{2500}$$

246 KJ/mol

249.49 KJ/mol

- in other words, our guess of 2500 K was too high
- we need choose a lower temperature and re-do the process until  $\Delta_r H^0 = \Delta H_{298}^{2500}$

This will ultimately give us the desired combustion temperature.

In your exam problems, you'll not be expected to perform the next iteration steps by hand, but I do want you to understand the significance of such calculations. We will need them in determining the performance of propulsion systems where such reactions are expected.