Advanced Combustion Engineering

Sources and Health Effects of Air Pollution

Pollutant	Sources	Health Effects
Ozone (O_3)	• Secondary pollutant formed by chemical reaction • Volatile organic compounds **(VOCs) + NOx** in the presence of **sunlight**.	• Decreases lung function and **lung diseases** • Causes respiratory symptoms (coughing and shortness of breath) • Aggravates **asthma** and other lung diseases
Particulate Matter (PM)	• Emitted or formed through chemical reactions • **Fuel combustion** (e.g., burning coal, wood, diesel) • **Industrial processes** • **Agriculture (plowing, field burning)** • **Unpaved roads.**	• **Heart or lung diseases** ➔ respiratory symptoms
Lead	• **Smelters (metal refineries)** • **Metal industries** • **Combustion of leaded gasoline in piston engine** • **Waste incinerators** • **Battery manufacturing**	• Damages the **nervous system** ➔ IQ loss and impacts on learning, memory, and behavior in children. • **Cardiovascular** and **renal** effects in adults
Oxides of Nitrogen (NO_x)	• **Fuel combustion** (e.g., electric utilities, industrial boilers, and vehicles) and wood burning.	• Aggravate **lung diseases** leading to respiratory symptoms
Carbon Monoxide (CO)	• **Fuel combustion** (especially vehicles).	• **Reduces the amount of oxygen** reaching the body's organs and tissues • Aggravates heart disease, resulting in chest pain and other symptoms leading to hospital admissions and ED visits.
Sulfur Dioxide (SO_2)	• **Fuel combustion** (especially high-sulfur coal); • Electric utilities and industrial processes • Natural sources such as **volcanoes**	• Aggravates **asthma** and increased respiratory symptoms. • Contributes to particle formation with associated health effects.

Basics of thermodynamics for combustion

(1) **Stoichiometry**: Mass balance calculations for chemical reactions

$$aA + bB \rightarrow cC + dD$$

where A, B, C, D : molecular species
a, b, c, d : stoichiometric coefficient

(2) **Generalized reaction** $\sum_{i=1}^{N} \nu_i{}' M_i \rightarrow \sum_{i=1}^{N} \nu_i{}'' M_i$

where, $M_i \equiv$ i-th of N molecular species
$\nu_i{}' \equiv$ stoichiometric coefficient of reactant
$\nu_i{}'' \equiv$ stoichiometric coefficient of products

Ex) Determine stoichiometric coefficient when 1 mole CH_4 is burned to form CO_2 and H_2O

$$CH_4 + 2O_2 \rightarrow 2\,H_2O + CO_2$$

Basics of thermodynamics for combustion

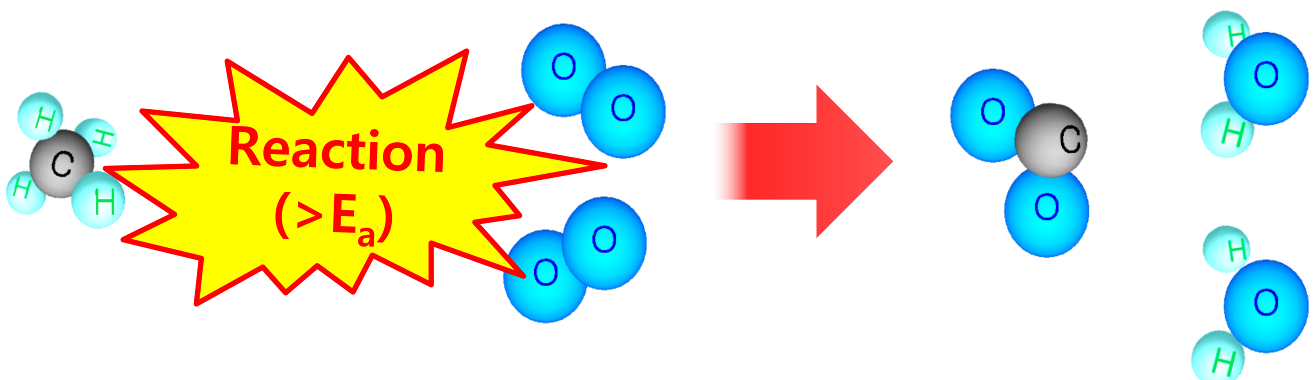
(3) Stoichiometric Reactions

– the most stable reaction in which all of the reactants are consumed.

$$CH_4 + 4O_2 \rightarrow 2O_2 + 2H_2O + CO_2$$ (Not stoi.)

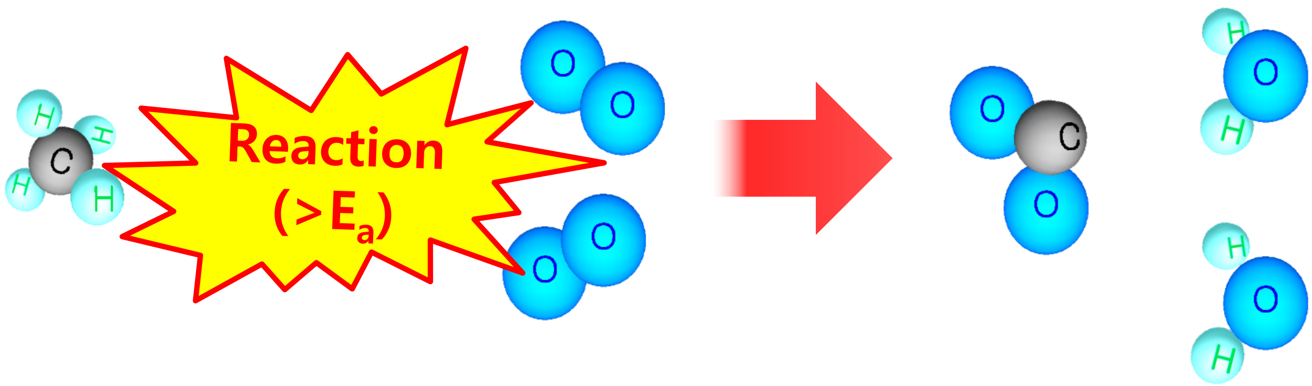
$$CH_4 + 1\frac{1}{2}O_2 \rightarrow 2H_2O + CO$$ (Not stoi.)

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$ (Stoichiometric)



Stoichiometric Reactions

❖ **Methane Reaction:** $CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2\,H_2O + 7.52N_2$



❖ **Equivalence Ratio:** $\phi \equiv \dfrac{F/A}{(F/A)_{stoi}} = \dfrac{(A/F)_{stoi}}{A/F} = \dfrac{1}{\lambda}$

>1, fuel rich (just "rich")

<1, fuel lean (just "lean")

❖ **Generalized Non-stoichiometric Reactions**

$$\varphi\, C_m H_n O_l + \frac{4m+n-2l}{4}(O_2 + 3.76N_2) \rightarrow \varphi\, m\, CO_2 + 0.5\,\varphi\, \mathrm{n}\, H_2O + (0.5\varphi\, l + 2 - 2\varphi)O_2 + 3.76\frac{4m+n-2l}{4}N_2$$

(4) Conventions for Fuel Mixtures

– the most stable reaction in which all of the reactants are consumed.

① Fuel / Oxidant Ratio (F/O) = mass of fuel/mass of oxidant

② Fuel / Air Ratio (F/A) = mass of fuel/mass of air

Ex) $2H_2 + O_2 \rightarrow$ Products

$$F/O = \left(2\,moles \times \frac{2g}{1mole}\right) \Big/ \left(1mole \times \frac{32g}{1mole}\right) = 0.125$$

$$F/A = \frac{(2\,moles \times 2g/1mole)}{(1mole\,of\;O_2)\left(\frac{32g}{1mole}\right) + (3.76\,mole\,of\;N_2)\left(\frac{28g}{1mole}\right)} = 0.029$$

③ Equivalence Ratio $\phi \equiv \frac{F/A}{(F/A)_{stoi}} = \frac{(A/F)_{stoi}}{A/F} = \frac{1}{\lambda}$

④ Air Excess Ratio $\lambda \equiv \frac{1}{\phi}$

>1, fuel rich (just "rich")

<1, fuel lean (just "lean")

=1, stoichiometric

Ex. 2.2

A NG-fired industrial boiler

$$Given: \chi_{O2} = 0.03, \quad MW_{air} = 28.85, \quad MW_{fuel} = 16.04$$

$$Find: AF \quad and \quad \phi$$

[Sol.]

$$CH_4 + a(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + bO_2 + 3.76aN_2$$

For O atom: 2a=2+2+2b ➔ b=a-2

$$\chi_{O2} = \frac{N_{O_2}}{N_{mix}} = \frac{b}{1+2+b+3.76a} = \frac{a-2}{1+4.76a} = 0.03 \quad \Rightarrow \quad a = 2.368$$

$$(AF) = \frac{N_{air}}{N_{fuel}} \frac{MW_{air}}{MW_{fuel}} = \frac{4.76a}{1} \frac{MW_{air}}{MW_{fuel}} = \frac{4.76(2.368)(28.85)}{16.04} = \underline{20.3}$$

$$(AF)_{stoi} = \frac{4.76(2)28.85}{16.04} = 17.1$$

$$\therefore \ \phi = \frac{(AF)_{stoi}}{(AF)} = \frac{17.1}{20.3} = \underline{0.84} \quad \text{[kg/kg]}$$

Basics of thermodynamics

(4) First Law of Thermodynamics

There exists an extensive function U called the internal energy having the property that for any closed system the heat added during any infinitesimal process is:

$$\delta Q = dU + \delta W$$
$$= dU + PdV$$

(5) Second Law of Thermodynamics

There exists an extensive function S such that for a closed system

$$dS \geq \frac{\delta Q}{T}$$

The equality holds for reversible processes.

Enthalpy of combustion & heating value

Enthalpy of combustion

$$q_{cv} - w_{cv} = (h_o - h_i) + \frac{1}{2}(v_o^2 - v_i^2) + g(z_o - z_i)$$

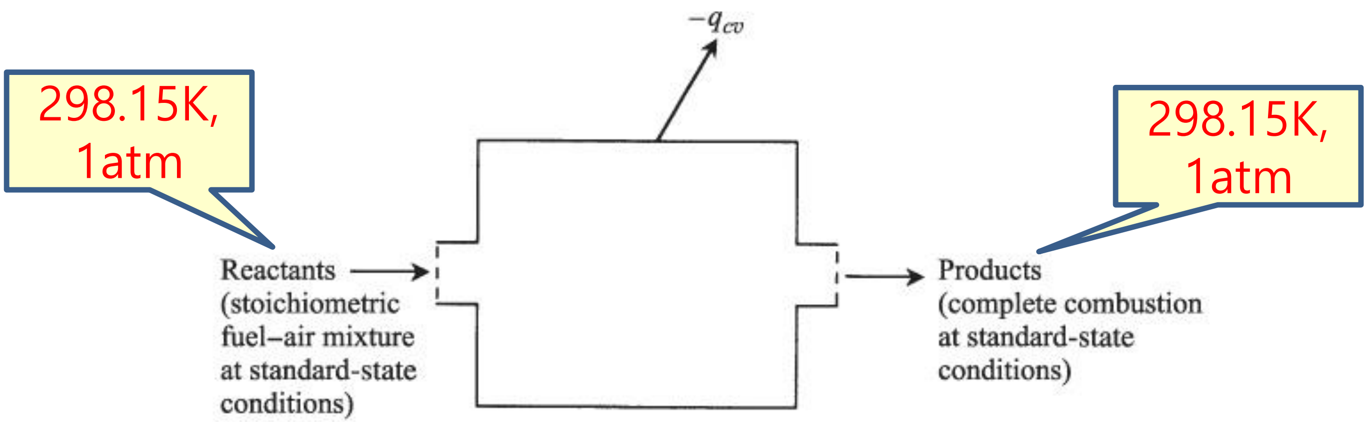


Figure 2.7 Steady-flow reactor used to determine enthalpy of combustion.

Ignore difference of kinetic and potential energy btw input and output, and assume no shaft work

Energy conservation: $q_{cv} = h_o - h_i = h_{prod} - h_{reac}$

Enthalpy of combustion: $\Delta h_R \equiv q_{cv} = h_{prod} - h_{reac}$
(Enthalpy of reaction)

Extensive property: $\Delta H_R = H_{prod} - H_{reac}$

Enthalpy of combustion & heating value

Heating value

Heat of combustion: (Heating value) $\Delta h_c = -\Delta h_R$ Enthalpy of combustion: (Enthalpy of reaction)

Higher Heating Value(HHV, Upper Heating Value): heat of combustion calculated assuming that **all of the water** in the products has condensed to liquid

Lower Heating Value(LHV): heat of combustion calculated assuming that **no water** in the products has condensed to liquid

cf) $HHV_{CH4} = LHV_{CH4} \times 111\%$

See appendix B