THE UNIVERSITY OF JORDAN

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Fuel and Energy

Material Balance
Part 3: Combustion Reactions

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Content

- ✓ Combustion Chemistry
- ✓ Theoretical and Excess Air
- ✓ Material Balances on Combustion Reactors

Type of fuels

1. Solid fuels

Coal, oil shale, biomass (carbon, some hydrogen and sulfur, and various noncombustible materials)

2. Liquid fuels

Fuel oil (mostly high molecular weight hydrocarbons, some sulfur)

3. Gaseous fuel

Natural gas, which is primarily methane, or liquefied petroleum gas, which is usually propane and/or butane.

When a fuel is burned

Carbon, C	$\longrightarrow$	CO_2 or CO
Hydrogen, H	$\longrightarrow$	H_2O
Sulfur, S	$\longrightarrow$	Sulfur, SO_2

- At temperatures greater than approximately 1800°C, some of the nitrogen (N) in the air reacts to form nitric acid (NO_x).
- A combustion reaction in which CO is formed from a hydrocarbon is referred to as partial combustion or incomplete combustion of the hydrocarbon.

$C + O_2 \rightarrow CO_2$	Complete combustion of carbon
$C_3H_8 + 5\,O_2 \rightarrow 3\,CO_2 + 4\,H_2O$	Complete combustion of propane
$C_3H_8 + \frac{7}{2}O_2 \rightarrow 3\,CO + 4\,H_2O$	Partial combustion of propane
$CS_2 + 3\,O_2 \rightarrow CO_2 + 2\,SO_2$	Complete combustion of carbon disulfide

- Air is the source of oxygen in most combustion reactors

N_2	78.03%
O_2	20.99%
Ar	0.94%
CO_2	0.03%
H_2, He, Ne, Kr, Xe	0.01%
	100.00%

Average molecular weight = 29.0

For simplicity, assume that the air consists of:

79% N_2, 21% O_2 $\Longrightarrow$ 79 moles N_2/21 moles O_2 = 3.76 moles N_2/mole O_2

- Composition on a wet basis is commonly used to denote the component mole fractions of a gas that contains water,
- Composition on a dry basis signifies the component mole fractions of the same gas without the water

It is important to be to convert a composition on a dry basis to its corresponding composition on a wet basis

- The product gas that leaves a combustion furnace is referred to as the stack gas, exhaust gas or flue gas.

Example

A stack gas contains 60.0 mole% N_2, 15.0% CO_2, 10.0% O_2, and the balance H_2O. Calculate the molar composition of the gas on a dry basis.

Example

An Orsat analysis (a technique for stack analysis) yields the following dry basis composition

N_2	65%	CO_2	14%	CO	11%	O_2	10%

A humidity measurement shows that the mole fraction of H_2O in the stack gas is 0.070. Calculate the stack gas composition on a wet basis.

Theoretical and Excess Air

- Combustion reactions are usually run with more air than is needed to supply oxygen in stoichiometric proportion to the fuel.
- This has the effect of increasing the conversion of the valuable reactant at the expense of the cost of the excess reactant and additional pumping costs.

- **Theoretical Oxygen:**

The moles (batch) or molar flow rate (continuous) of O_2 needed for complete combustion of all the fuel fed to the reactor, assuming that all carbon in the fuel is oxidized to CO_2 and all the hydrogen is oxidized to H_2O

- Theoretical Air: The quantity of air that contains the theoretical oxygen.

- **Excess Air:**

The amount by which the air fed to the reactor exceeds the theoretical air

Percent Excess Air:

$$\frac{(\text{moles air})_{\text{fed}} - (\text{moles air})_{\text{theoretical}}}{(\text{moles air})_{\text{theoretical}}} \times 100\%$$

If 50% excess air is supplied

$$(\text{moles air})_{\text{fed}} = 1.5\,(\text{moles air})_{\text{theoretical}}$$

Example

One hundred mol/h of butane (C_4H_{10}) and 5000 mol/h of air are fed into a combustion reactor. Calculate the percent excess air.

The stoichiometric equation for complete combustion of butane:

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4\,CO_2 + 5\,H_2O$$

The theoretical air from the feed rate of fuel and the stoichiometric equation

$$(\dot{n}_{O_2})_{\text{theoretical}} = \frac{100 \text{ mol } C_4H_{10}}{\text{h}} \left| \frac{6.5 \text{ mol } O_2 \text{ required}}{\text{mol } C_4H_{10}} \right. = 650 \ \frac{\text{mol } O_2}{\text{h}}$$

$$(\dot{n}_{\text{air}})_{\text{theoretical}} = \frac{650 \text{ mol } O_2}{\text{h}} \left| \frac{4.76 \text{ mol air}}{\text{mol } O_2} \right. = 3094 \ \frac{\text{mol air}}{\text{h}}$$

$$\% \text{ excess air} = \frac{(\dot{n}_{\text{air}})_{\text{fed}} - (\dot{n}_{\text{air}})_{\text{theoretical}}}{(\dot{n}_{\text{air}})_{\text{theoretical}}} \times 100\% = \frac{5000 - 3094}{3094} \times 100\% = \boxed{61.6\%}$$

$$(\dot{n}_{\text{air}})_{\text{fed}} = 1.616(\dot{n}_{\text{air}})_{\text{theoretical}} = 1.616(3094 \text{ mol/h}) = 5000 \text{ mol/h}.$$

Material Balances on Combustion Reactors

Example

Ethane is burned with 50% excess air. The percentage conversion of the ethane is 90%; of the ethane burned. 25% reacts to form CO and the balance reacts to form CO_2. Calculate the molar composition of the stack gas on a dry basis and the mole ratio of water to dry stack gas.

$$C_2H_6 + \quad O_2 \longrightarrow \quad CO_2 + \quad H_2O$$

$$C_2H_6 + \quad O_2 \longrightarrow \quad CO + \quad H_2O$$

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Example

A hydrocarbon gas is burned with air. The dry-basis product gas composition is 1.5 mole% CO, 6.0% CO_2, 8.2% O_2, and 84.3% N_2. There is no atomic oxygen in the fuel. Calculate the ratio of hydrogen to carbon in the fuel gas and speculate on what the fuel might be. Then calculate the percent excess air fed to the reactor.