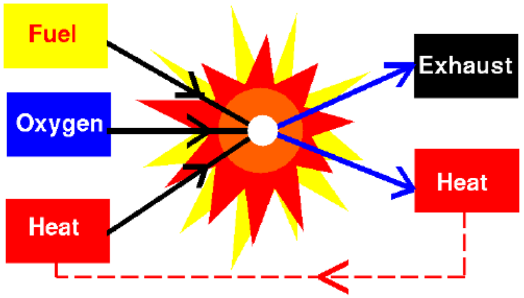
CHAPTER 4.7



Balances on Reactive Process Combustion Reaction

Combustion Reaction

Rapid oxidation of a fuel accompanied by the release of heat and/or light together with the formation of combustion products

Fuel + oxidant ➡ heat/light + combustion products

Definition of combustion as quoted from Webster's dictionary

"rapid oxidation generating heat, or both heat and light ; also, slow oxidation accompanied by relatively little heat and no light"

Combustion of Fossil Fuel

Chemical reaction between hydrogen and carbon atoms (contained in the fuel) with oxygen atoms (usually comes from the air), resulting in the heat release and the formation of combustion products(*)

(*) mainly water vapor and carbon dioxide and a certain amount combustion by-products depending on combustion process

Simplified Main Processes of Combustion

Carbon + Oxygen ➡ heat + carbon dioxide

$(C + O_2 \rightarrow Heat + CO_2)$

Hydrogen + Oxygen ➡ Heat + Water

$(H_2 + \frac{1}{2} O_2 \rightarrow Heat + H_2O)$

Combustion By-Products

Carbon monoxide (CO)
Aldehydes (e.g. H)
Unburned Fuel
Radicals

} mainly due to incomplete combustion

Oxides of nitrogen (NOx) – reaction between O_2 (in air) and nitrogen (present in air or fuel)

Oxides of sulphur (SOx) – only for Sulphur-containing fuel

Categories of Combustion Process

- Complete combustion
  - ✓ Stoichiometric
  - ✓ Excess air or fuel lean
- Incomplete or partial combustion
  - ✓ Excess fuel or fuel rich or deficient air

In practice, combustion will never be complete even though at stoichiometric or excess air conditions…… due to **non-uniformity of fuel and air mixture** and **complexity of combustion reaction**

Source of Oxygen

- Main of source of oxygen comes from atmospheric air
- Atmospheric air requirement for combustion reaction is assumed to have the following composition

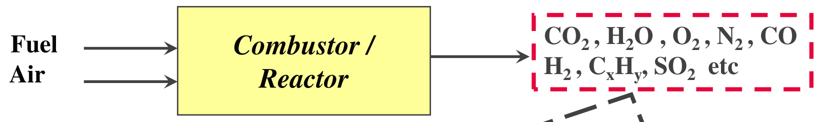
Air %	By volume	By weight (mass)
O_2	21	23
N_2	79	77

- Analyses of solid / liquid fuels are normally reported on a mass basis, while gaseous fuels are normally analysed on a volume basis

Composition analysis

Fuel composition analysis – conversion from a composition by mass to a molar composition or vice-versa (refer to page 51 in the textbook)

Stack or flue gases composition analysis



Wet basis composition :- component mole fractions of gas with the presence of water

Dry basis composition :- component mole fractions of the same gas without the presence of water

Theoretical and Excess Oxygen (Air)

Theoretical Oxygen (air)

The amount of chemically-corrected (stoichiometric) amount of oxygen (air) required for complete combustion of a given quantity of a specific fuel)

Excess Oxygen (Air)

The actual amount of oxygen (air) required for combustion of a specific fuel

The theoretical oxygen (air) required to burn a given quantity of fuel does not depend on how much fuel is actually burned. The fuel may not react completely and it may react to form both CO and CO_2, but the theoretical air is still that which would be required to react with all of the fuel to form CO_2 only.

Percent theoretical Oxygen (Air)

$$\frac{(\text{moles oxygen})_{\text{required}} - (\text{moles oxygen})_{\text{theoretical}}}{(\text{moles oxygen})_{\text{theoretical}}} \times 100\%$$

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

The value of the percent excess air depends on the theoretical air and the air feed rate - **not much oxygen is consumed** in the reactor or whether **combustion is complete** or partial

Example 1

Theoretical and Excess Oxygen (Air)

100 mol/h methane is fed to a reactor and burns in the reaction

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

$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$

a) What is the theoretical O_2 flow rate if the complete combustion occurs in the reactor?
b) What is the theoretical O_2 flow rate if only 70% of the methane reacts?
c) What is the theoretical air flow rates?
d) If 100% excess air is supplied, what is the flow rate of air entering the reactor?
e) If the actual flow rates of air is such that 300 mol/h O_2 enters the reactor , what is the percent excess air?

Solution - Example 1

1/2

Theoretical and Excess Oxygen (Air)

100 mol/h methane is fed to a reactor and burns in the reaction

a) What is the theoretical O_2 flow rate if the complete combustion occurs in the reactor?

b) What is the theoretical O_2 flow rate if only 70% of the methane reacts?

Solution - Example 1 2/2

Theoretical and Excess Oxygen (Air)

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c) What is the theoretical air flow rates?

d) If 100% excess air is supplied, what is the flow rate of air entering the reactor?

e) If the actual flow rates of air is such that 300 mol/h O_2 enters the reactor , what is the percent excess air?

Material Balances Involving Combustion Reaction

- The procedures for writing and solving material balances for a combustion reactor is the same as that for any other reactive system.
- **Unlike material balances on non-reactive processes, you cannot automatically assume the total moles of the reactants equal to that of the products (i.e. moles input = moles output)**

  General balance on reactive system : Input + Generation = Output + Consumption

- What information should be in a process flow chart?
  - Inlet stream components
    - ✓ Fuel (single or mixture)
    - ✓ Oxygen or Air (21 mole % oxygen, 79 mole% nitrogen)
    - ✓ Excess oxygen or air (percent excess oxygen or air that is required or already given)
  - Outlet stream components
    - ✓ CO_2, H_2O and CO (if combustion is partially complete)
    - ✓ Un-reacted fuel (if fuel not fully consumed)
    - ✓ Un-reacted O_2 (depends on combustion reaction or excess air)
    - ✓ N_2 (if oxygen comes from air)

Material Balances Involving Combustion Reaction

- Percentage of excess oxygen and excess air would have the same value.
  - ✓ Calculate **the theoretical amount of oxygen or air required for a given amount fuel to produce complete combustion,** ***eventhough the actual combustion reaction is not complete*****…..** (write stoichiometric balance of fuel-oxygen combustion to form CO_2 and H_2O)
  - ✓ Multiply the theoretical amount of oxygen or air with the excess air fraction (i.e 1 + fractional excess oxygen or air)
- Which mass balance method is preferred?
  - ✓ If only one reaction is involved, all three balance methods (molecular species, atomic species or extent of reaction) are equally convenient.
  - ✓ If more than one reaction is involved simultaneously, atomic species balances is usually more convenient.

Example 2

Combustion reaction of a mixture of hydrocarbon fuels

A mixture of hydrocarbon gases containing , on a volume basis, 95 mole % methane, 2 mole % propane and 3 mole % nitrogen is completely burned with 30 mole % excess air. Calculate the molar composition of combustion products on a dry and wet basis

Basis : 100 mol of fuel mixture

Strategy : Solve the unknowns from the given information.

n_o mol Air (30% Excess)

Nitrogen balance

CO_2 balance

H_2O balance

O_2 balance

Example 3

Partial/Incomplete combustion

Combustion of methane can be presented by the following reactions;

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$

100 mol/h of methane is fed to a reactor and completely burns with 50% excess air. The analysis of the flue gases indicates that the mole ratio of CO_2 to CO is 3. Calculate the molar composition of the flue gases on a wet basis.

Process flow diagram:

Basis : 100 mol/h of methane

Strategy : Solve the unknowns from the given information.

Theoretical Air

Percent excess air (50%)

Nitrogen balance

Atomic Hydrogen balance

Atomic Carbon balance

Solution – Example 3 5/6

Atomic Oxygen balance

Solution – Example 3 6/6

Composition of flue gas (wet basis) :

Example 4

Analysis of combustion products

Methane is burned with atmospheric air in a combustor. The analysis of the combustion products on a dry basis is as follows;

CO_2	10.00 %
O_2	2.37 %
CO	0.53 %
N_2	87.10 %

Calculate

a. the molar composition of combustion products on a wet basis.
b. the percentage of excess air required.
c. the fractional conversion of methane to carbon dioxide
d. the fractional conversion of methane to carbon monoxide.

Solution – Example 4 1/4

Basis :

Process flow diagram

Solution – Example 4 2/4

Strategy : Solve the unknowns from the given information.

Nitrogen balance

Atomic Carbon balance

Solution – Example 4 3/4

Theoretical Air

Atomic Hydrogen

Solution – Example 4 4/4

The molar composition of combustion products on a wet basis :

Percentage of excess air :

Fractional conversion of methane to CO & CO_2 :

Example 5

Ethane is initially mixed with oxygen to obtain gas containing 80% C_2H_6 and 20% O_2 that is then burned in an engine with 200% excess air. 80% of ethane turns to CO_2, 10% to CO and the rest remains unburned. Calculate the composition (mole %) of the exhaust gas on a wet and dry basis.

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