Combustion

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1 Introduction

Flame resulting from the combustion (burning) of a fuel

Combustion or burning is a complex sequence of exothermic chemical reactions between a fuel and an oxidant accompanied by the production of heat or both heat and light in the form of either a glow or flames. Direct combustion by atmospheric oxygen is a reaction mediated by radical intermediates. The conditions for radical production are naturally produced by thermal runaway, where the heat generated by combustion is necessary to maintain the high temperature necessary for radical production. In a complete combustion reaction, a compound reacts with an oxidizing element, such as oxygen or fluorine, and the products are compounds of each element in the fuel with the oxidizing element.

For example:
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
$CH_2S + 6F_2 \rightarrow CF_4 + 2HF + SF_6$

A simpler example can be seen in the combustion of hydrogen and oxygen, which is a commonly used reaction in rocket engines:

$2H_2 + O_2 \rightarrow 2H_2O + \text{heat}$

The result is simply water vapor.
In the large majority of the real world uses of combustion, the oxygen (O 2) oxidant is obtained from the ambient air and the resultant flue gas from the combustion will contain nitrogen:

$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2 + \text{heat}$

As can be seen, when air is the source of the oxygen, nitrogen is by far the largest part of the resultant flue gas. In reality, combustion processes are never perfect or complete. In flue gases from combustion of carbon (as in coal combustion) or carbon compounds (as in combustion of hydrocarbons, wood etc.) both unburned carbon (as soot) and carbon compounds (CO and others) will be present. Also, when air is the oxidant, some nitrogen will be oxidized to various nitrogen oxides (NO_x).

2 Types of combustion

2.1 Rapid

Rapid combustion is a form of combustion in which large amounts of heat and light energy are released, which often results in a fire. This is used in a form of machinery such as internal combustion engines and in thermobaric weapons.

2.2 Slow

Slow combustion is a form of combustion which takes place at low temperatures. Cellular respiration is an example of slow combustion.

2.3 Complete

In complete combustion, the reactant will burn in oxygen, producing a limited number of products. When a hydrocarbon burns in oxygen, the reaction will only yield carbon dioxide and water. When a hydrocarbon or any fuel burns in air, the combustion products will also include nitrogen. When elements such as carbon, nitrogen, sulfur, and iron are burned, they will yield the most common oxides. Carbon will yield carbon dioxide. Nitrogen will yield nitrogen dioxide. Sulfur will yield sulfur dioxide. Iron will yield iron(III) oxide. It should be noted that complete combustion is almost impossible to achieve. In reality, as actual combustion reactions come to equilibrium, a wide variety of major and minor species will be present. For example, the combustion of methane in air will yield, in addition to the major products of carbon dioxide and water, the minor product carbon monoxide and nitrogen oxides, which are products of a side reaction (oxidation of nitrogen).

2.4 Turbulent

Turbulent combustion is a combustion characterized by turbulent flows. It is the most used for industrial application (e.g. gas turbines, diesel engines, etc.) because the turbulence helps the mixing process between the fuel and oxidizer.

2.5 Incomplete

Incomplete combustion occurs when there isn't enough oxygen to allow the fuel (usually a hydrocarbon) to react completely with the oxygen to produce carbon dioxide and water, also when the combustion is quenched by a heat sink such as a solid surface or flame trap. When a hydrocarbon burns in air, the reaction will yield carbon dioxide, water, carbon monoxide, pure carbon (soot or ash) and various other compounds such as nitrogen oxides.

The quality of combustion can be improved by design of combustion devices, such as burners and internal combustion engines. Further improvements are achievable by catalytic after-burning devices (such as catalytic converters) or by the simple partial return of the exhaust gases into the combustion process. Such devices are required by environmental legislation for cars in most countries, and may be necessary in large combustion devices, such as thermal power plants, to reach legal emission standards.

2.6 Smoldering

Smouldering combustion is a flameless form of combustion, deriving its heat from heterogeneous reactions occurring on the surface of a solid fuel when heated in an oxidizing environment. The fundamental difference between smouldering and flaming combustion is that in smouldering, the oxidation of the reactant species occurs on the surface of the solid rather than in the gas phase. The characteristic temperature and heat released during smoldering are low compared to those in the flaming combustion of a solid. Typical values in smouldering are around 600 °C for the peak temperature and 5 kJ/g-O_2 for the heat released; typical values during flaming are around 1500 °C and 13 kJ/g-O_2 respectively. These characteristics cause smoulder to propagate at low velocities, typically around 0.1 mm/s, which is about two orders of magnitude lower than the velocity of flame spread over a solid. In spite of its weak combustion characteristics, smouldering is a significant fire hazard.

3 Combustion with other oxidants

Oxygen can be assumed as the oxidant when talking about combustion, but other oxidants exist. Nitrous oxide is used in rockets and in motorsport; it produces oxygen at over 1300 C. Fluorine, another oxidizing element, can produce a combustion reaction, to produce fluorinated products (rather than oxides). For example, mixtures of gaseous fluorine and methane are explosive, just like mixtures of oxygen and methane. Chlorine trifluoride is a strong fluorinating agent that ignites fuels more readily than oxygen.

4 Chemical equation

Generally, the chemical equation for stoichiometric burning of hydrocarbon in oxygen is as follows:

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow \; xCO_2 + \left(\frac{y}{2}\right) H_2O$$

For example, the burning of propane is:

$$C_3H_8 + 5O_2 \rightarrow \; 3CO_2 + 4H_2O$$

The simple word equation for the combustion of a hydrocarbon in oxygen is:

$$\text{Fuel} + \text{Oxygen} \rightarrow \; \text{Heat} + \text{Water} + \text{Carbon dioxide}$$

If the combustion takes place using air as the oxygen source, the nitrogen can be added to the equation, although it does not react, to show the composition of the flue gas:

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 + 3.76 \left(x + \frac{y}{4}\right) N_2 \rightarrow \; xCO_2 + \left(\frac{y}{2}\right) H_2O + 3.76 \left(x + \frac{y}{4}\right) N_2$$

For example, the burning of propane is:

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow \; 3CO_2 + 4H_2O + 18.8N_2$$

The simple word equation for the combustion of a hydrocarbon in air is:

$$\text{Fuel} + \text{Air} \rightarrow \; \text{Heat} + \text{Water} + \text{Carbon dioxide} + \text{Nitrogen}$$

Nitrogen may also oxidize when there is an excess of oxygen. The reaction is thermodynamically favored only at high temperatures. Diesel engines are run with an excess of oxygen to combust small particles that tend to form with only a stoichiometric amount of oxygen, necessarily producing nitrogen oxide emissions. Both the United States and

European Union are planning to impose limits to nitrogen oxide emissions, which necessitate the use of a special catalytic converter or treatment of the exhaust with urea.

5 Fuels

5.1 Liquid fuels

Combustion of a liquid fuel in an oxidizing atmosphere actually happens in the gas phase. It is the vapour that burns, not the liquid. Therefore, a liquid will normally catch fire only above a certain temperature, its flash point. The flash point of a liquid fuel is the lowest temperature at which it can form an ignitable mix with air. It is also the minimum temperature at which there is enough evaporated fuel in the air to start combustion.

5.2 Solid fuels

The act of combustion consists of three relatively distinct but overlapping phases:

- Preheating phase, when the unburned fuel is heated up to its flash point and then fire point. Flammable gases start being evolved in a process similar to dry distillation.
- Distillation phase or gaseous phase, when the mix of evolved flammable gases with oxygen is ignited. Energy is produced in the form of heat and light. Flames are often visible. Heat transfer from the combustion to the solid maintains the evolution of flammable vapours.
- Charcoal phase or solid phase, when the output of flammable gases from the material is too low for persistent presence of flame and the charred fuel does not burn rapidly anymore but just glows and later only smoulders.

6 Temperature

Assuming perfect combustion conditions, such as complete combustion under adiabatic conditions (i.e., no heat loss or gain), the adiabatic combustion temperature can be determined. The formula that yields this temperature is based on the first law of thermodynamics and takes note of the fact that the heat of combustion is used entirely for heating the fuel, the combustion air or oxygen, and the combustion product gases (commonly referred to as the flue gas).

In the case of fossil fuels burnt in air, the combustion temperature depends on

- the heating value
- the stoichiometric air to fuel ratio λ
- the specific heat capacity of fuel and air
- the air and fuel inlet temperatures

The adiabatic combustion temperature (also known as the adiabatic flame temperature) increases for higher heating values and inlet air and fuel temperatures and for stoichiometric air ratios approaching one.

Most commonly, the adiabatic combustion temperatures for coals are around 2200 °C (for inlet air and fuel at ambient temperatures and for $\lambda = 1.0$), around 2150 °C for oil and 2000 °C for natural gas.

In industrial fired heaters, power plant steam generators, and large gas-fired turbines, the more common way of expressing the usage of more than the stoichiometric combustion air is percent excess combustion air. For example, excess combustion air of 15 percent means that 15 percent more than the required stoichiometric air is being used.

7 Combustion analysis

This section provides a combustion analysis for a few typical fuels (carbon, hydrogen, sulfur, coal, oil and gas) when the fuel reacts with air at stoichiometric conditions. For this analysis, both fuel and air are taken to be at inlet combustion conditions of 298 K and 1 atm of absolute pressure, and combustion is taken to be complete and with no heat loss.

The analysis also requires knowing the physical properties for the reactants and combustion products, as well as knowing the composition of both the fuel and oxidant compositions. For solid and liquid type fuels, the fuel compositions is given on weight fraction basis. In this analysis, CH_4 is the only gas fuel considered. In order to keep the combustion analysis simple and straightforward, the CH_4 composition is also provided on the weight fraction basis. Oxidant composition is usually given on the mole or volume basis.

Table 1 provides some fuel compositions on a weight fraction basis:

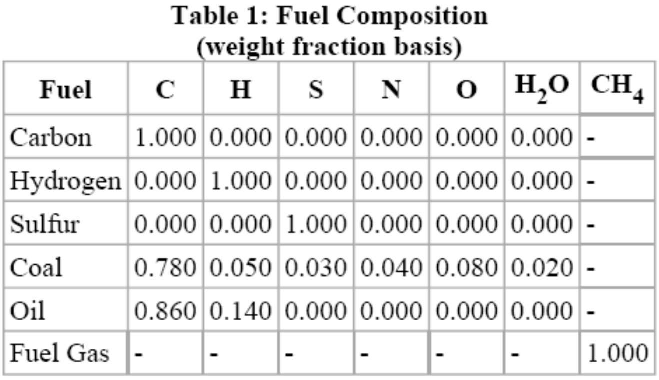

Table 1: Fuel Composition (weight fraction basis)

Fuel	C	H	S	N	O	H_2O	CH_4
Carbon	1.000	0.000	0.000	0.000	0.000	0.000	-
Hydrogen	0.000	1.000	0.000	0.000	0.000	0.000	-
Sulfur	0.000	0.000	1.000	0.000	0.000	0.000	-
Coal	0.780	0.050	0.030	0.040	0.080	0.020	-
Oil	0.860	0.140	0.000	0.000	0.000	0.000	-
Fuel Gas	-	-	-	-	-	-	1.000

Table 2 provides the composition of air:

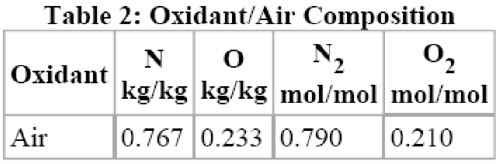

Table 2: Oxidant/Air Composition

Oxidant	N kg/kg	O kg/kg	N_2 mol/mol	O_2 mol/mol
Air	0.767	0.233	0.790	0.210

Again, in this combustion analysis, only the stoichiometric combustion is analyzed. Results of such analysis are provided, including the composition of the combustion gas products on a weight and mole/volume basis, the adiabatic flame temperature, the stoichiometric ratio and the fuel's higher heating value (HHV).

Table 3 provides the composition of the combustion gas products on a weight fraction basis:

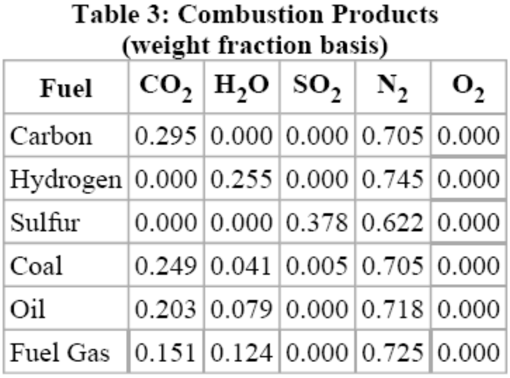

Table 3: Combustion Products (weight fraction basis)

Fuel	CO_2	H_2O	SO_2	N_2	O_2
Carbon	0.295	0.000	0.000	0.705	0.000
Hydrogen	0.000	0.255	0.000	0.745	0.000
Sulfur	0.000	0.000	0.378	0.622	0.000
Coal	0.249	0.041	0.005	0.705	0.000
Oil	0.203	0.079	0.000	0.718	0.000
Fuel Gas	0.151	0.124	0.000	0.725	0.000

Table 4 provides the composition of the combustion gas products on a mole fraction basis (which is the same as a volume basis):

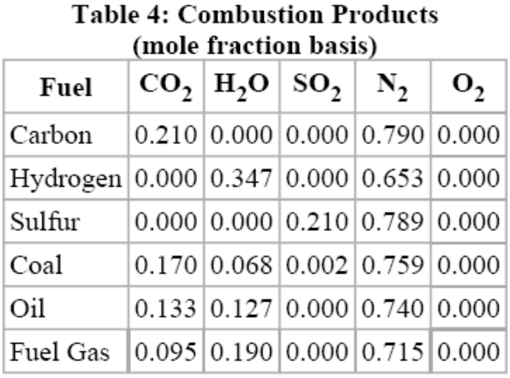

Table 4: Combustion Products (mole fraction basis)

Fuel	CO_2	H_2O	SO_2	N_2	O_2
Carbon	0.210	0.000	0.000	0.790	0.000
Hydrogen	0.000	0.347	0.000	0.653	0.000
Sulfur	0.000	0.000	0.210	0.789	0.000
Coal	0.170	0.068	0.002	0.759	0.000
Oil	0.133	0.127	0.000	0.740	0.000
Fuel Gas	0.095	0.190	0.000	0.715	0.000

When considering coal, oil and gas as the fuel, coal has the largest amount of CO 2 in the combustion gas products on both a weight and mole basis.

Table 5 provides the combustion adiabatic flame temperature, stoichiometric ratio and the fuel's higher heating value:

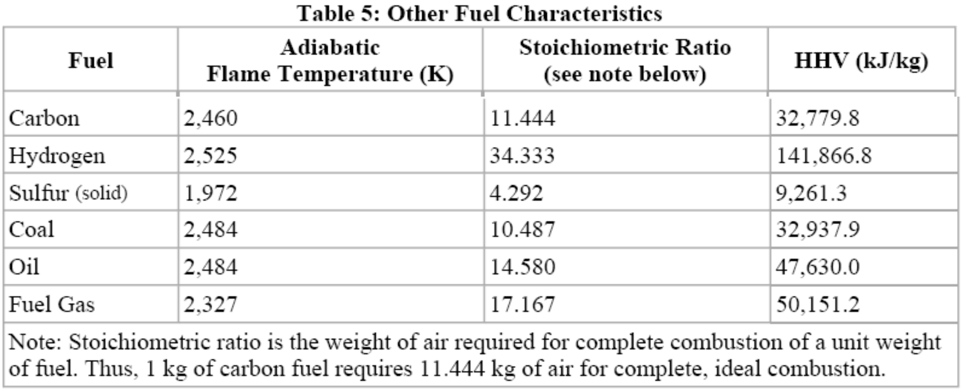

Table 5: Other Fuel Characteristics

Fuel	Adiabatic Flame Temperature (K)	Stoichiometric Ratio (see note below)	HHV (kJ/kg)
Carbon	2,460	11.444	32,779.8
Hydrogen	2,525	34.333	141,866.8
Sulfur (solid)	1,972	4.292	9,261.3
Coal	2,484	10.487	32,937.9
Oil	2,484	14.580	47,630.0
Fuel Gas	2,327	17.167	50,151.2

Note: Stoichiometric ratio is the weight of air required for complete combustion of a unit weight of fuel. Thus, 1 kg of carbon fuel requires 11.444 kg of air for complete, ideal combustion.

8 Instabilities

Combustion instabilities are typically violent pressure oscillations in a combustion chamber. These pressure oscillations can be as high as 180dB, and long term exposure to these cyclic pressure and thermal loads reduces the life of engine components. In rockets, such as the F1 used in the Saturn V program, instabilities led to massive damage of the combustion chamber and surrounding components. This problem was solved by re-designing the fuel injector. In liquid jet engines the droplet size and distribution can be used to attenuate the instabilities. Combustion instabilities are a major concern in ground-based gas turbine engines because of NOx emissions. The tendency is to run lean, an equivalence ratio less than 1, to reduce the combustion temperature and thus reduce the NO_x emissions; however, running the combustor lean makes it very susceptible to combustion instabilities.

The Rayleigh Criterion is the basis for analysis of thermoacoustic combustion instabilities and is evaluated using the Rayleigh Index over one cycle of instability.

$$G(x) = \frac{1}{T}\int_T q'(x,t)p'(x,t)dt$$

When the heat release oscillations are in phase with the pressure oscillations the Rayleigh Index is positive and the magnitude of the thermoacoustic instability increases. Consecutively if the Rayleigh Index is negative then thermoacoustic damping occurs. The Rayleigh Criterion implies that a thermoacoustic instability can be optimally controlled by having heat release oscillations 180 degrees out of phase with pressure oscillations at the same frequency. This minimizes the Rayleigh Index.

9 External links

- Hydrocarbon combustion (http://www25.brinkster.com/denshade/hydro.html) Simple applet that illustrates the Chemical equation.
- Fuel efficiency (stoichiometric air fuel mixture) vs. decreased emissions in combustion engines (http://www.normanchigier.com/Fuel_Injection_email.html)
- Combustion Analysis (http://www.habmigern2003.info/) The principles of exhaust fume analysis for assessing combustion quality in boilers.
- Simulation of gas combustion (http://mark.jelezniak.de/Chemked/index.htm)

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