Internal combustion engines

[redacted]

Chapter Four

Thermo-chemistry and Fuels

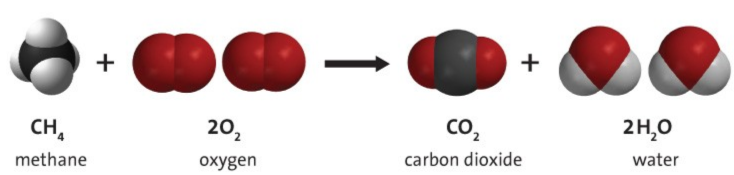
By

Laith Batarseh

Thermo-chemistry and Fuels

[redacted]

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



Isooctane	$C_8H_{18} + 12.5\ O_2 \rightarrow 8CO_2 + 9H_2O$

Thermo-chemistry and Fuels

Molecules react with molecules

where: m = mass
N = number of moles
M = molecular weight

In SI units:

$$1 \text{ kgmole of } CH_4 = 16.04 \text{ kg}$$

$$1 \text{ kgmole of } O_2 = 32.00 \text{ kg}$$

$$1 \text{ kgmole} = 6.02 \times 10^{26} \text{ molecules}$$

In English units:

$$1 \text{ lbmmole of } CH_4 = 16.04 \text{ lbm}$$

$$1 \text{ lbmmole of } O_2 = 32.00 \text{ lbm}$$

$$1 \text{ lbmmole} = 2.73 \times 10^{26} \text{ molecules}$$

Thermo-chemistry and Fuels

Air components

78% nitrogen by mole
21 % oxygen
1% argon
traces of C02, Ne, CH4, He, H20, etc.

Stoichiometric combustion of methane with *air is then:*

$$CH_4 + 2O_2 + 2(3.76)\,N_2 \rightarrow C0_2 + 2H_20 + 2(3.76)\,N_2$$

and of isooctane with air is:

$$C_8H_{18} + 12.5\,0_2 + 12.5(3.76)\,N_2 \rightarrow 8C0_2 + 9H_20 + 12.5(3.76)\,N_2$$

Thermo-chemistry and Fuels

stoichiometric

Combustion can occur, within limits, when more than stoichiometric air is present (lean) or when less than stoichiometric air is present (rich) for a given amount of fuel. If methane is burned with 150% stoichiometric air, the excess oxygen ends up in the products:

$$CH_4 + 3\,O_2 + 3(3.76)\,N_2 \rightarrow CO_2 + 2\,H_2O + 3(3.76)\,N_2 + O_2$$

If isooctane is burned with 80% stoichiometric air, there is not enough oxygen to convert all the carbon to CO_2, and carbon monoxide CO is found in the products:

$$C_8H_{18} + 10\,O_2 + 10(3.76)\,N_2 \rightarrow 3\,CO_2 + 9\,H_2O + 5\,CO + 10(3.76)\,N_2$$

TABLE 4-1 MOLECULAR WEIGHTS

SUBSTANCE		MOLECULAR WEIGHT (kg/kgmole) or (lbm/lbmmole)
Air		28.97
Argon	Ar	39.95
Carbon	C	12.01
Carbon Monoxide	CO	28.01
Carbon Dioxide	CO_2	44.01
Hydrogen	H_2	2.02
Water Vapor	H_2O	18.02
Helium	He	4.00
Nitrogen	N_2	28.01

Thermo-chemistry and Fuels

Various terminology is used for the amount of air or oxygen used in combustion.

80% stoichiometric air = 80% theoretical air = 80% air
= 20% deficiency of air

133% stoichiometric oxygen = 133% theoretical oxygen
= 133% oxygen = 33% excess oxygen

For actual combustion in an engine, the equivalence ratio is a measure of the fuel-air mixture relative to stoichiometric conditions. It is defined as:

$$\phi = (FA)_{act}/(FA)_{stoich} = (AF)_{stoich}/(AF)_{act} \qquad (4\text{-}2)$$

where: FA = m_f/m_a = fuel–air ratio
AF = m_a/m_f = air–fuel ratio
m_a = mass of air
m_f = mass of fuel

when:

$\phi < 1$ running lean, oxygen in exhaust

$\phi > 1$ running rich, CO and fuel in exhaust

$\phi = 1$ stoichiometric, maximum energy released from fuel

SI engines normally operate with an equivalence ratio in the range of 0.9 to 1.2, depending on the type of operation.

Thermo-chemistry and Fuels

EXAMPLE PROBLEM 4-1

Isooctane is burned with 120% theoretical air in a small three-cylinder turbocharged automobile engine.
Calculate:

1. air–fuel ratio
2. fuel–air ratio
3. equivalence ratio

Stoichiometric reaction:

$$C_8H_{18} + 12.5\ O_2 + 12.5(3.76)\ N_2 \rightarrow 8\ CO_2 + 9\ H_2O + 12.5(3.76)\ N_2$$

With 20% excess air:

$$C_8H_{18} + 15\ O_2 + 15(3.76)\ N_2 \rightarrow 8\ CO_2 + 9\ H_2O + 15(3.76)\ N_2 + 2.5\ O_2$$

With 20% excess air, all the fuel gets burned, and the same amount of CO_2 and H_2O is found in the products. In addition, there is some oxygen and additional nitrogen in the products (the excess air).

1) Equations (2-55) and (4-1) are used to find the air–fuel ratio:

$$AF = m_a/m_f = N_aM_a/N_fM_f = [(15)(4.76)(29)]/[(1)(114)]$$
$$= \underline{18.16}$$

Thermo-chemistry and Fuels

2) Equation (2-56) is used to find fuel–air ratio:

$$FA = m_f/m_a = 1/AF = 1/18.16 = \underline{0.055}$$

3) Fuel–air ratio of stoichiometric combustion:

$$(FA)_{stoich} = [(1)(114)]/[(12.5)(4.76)(29)] = 0.066$$

Equivalence ratio is obtained using Eq. (4-2):

$$\phi = (FA)_{act}/(FA)_{stoich} = (0.055)/(0.066) = \underline{0.833}$$