Northern Technical University
Engineering Technical College / Mosul
Power Mechanics Engineering Technology
Branch :Renewable Energy Engineering
Combustion Engineering Lectures

Fourth Year

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References:

1- turns-an_introduction_to_combustion
2- Engineering Fundamentals of IC
3- Stephen R. Turns-An Introduction to Combustion_ Concepts and Applications-McGraw-Hill (2000)

Lecture No(1)

Thermodynamic of combustion

1. Class : third Year
2. Subject : Thermodynamic of combustion
3. Number of weeks: one week
4. Central idea : Study Thermodynamic of combustion
5. The Test:

REVIEW OF PROPERTY RELATIONS

Equation of State

An **equation of state** provides the relationship among the pressure, P, temperature, T, and volume V (or specific volume v) of a substance. For ideal-gas behavior, i.e., a gas that can be modeled by neglecting intermolecular forces and the volume of the molecules, the following equivalent forms of the equation of state apply:

$$PV = NR_uT, \tag{1a}$$

$$PV = mRT, \tag{1b}$$

$$Pv = RT, \tag{1c}$$

or

$$P = \rho RT, \tag{1d}$$

where the specific gas constant R is related to the universal gas constant R_u (= 8315 J/kmol-K) and the gas molecular weight MW by

$$R = R_u/MW. \tag{2}$$

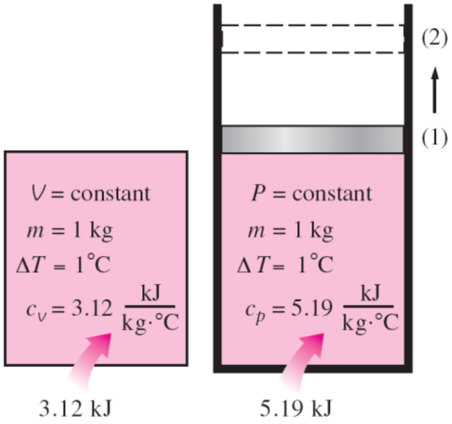
The density ρ in Eqn. 2.2d is the reciprocal of the specific volume ($\rho = 1/v = m/V$). Throughout this book, we assume ideal-gas behavior for all gaseous species and gas mixtures. This assumption is appropriate for nearly all of the systems we wish to consider since the high temperatures associated with combustion generally result in sufficiently low densities for ideal-gas behavior to be a reasonable approximation.

Specific Heat

Specific heat is defined as the amount of energy needed to increase the temperature of a unit mass of a substance by one degree. In thermodynamics, we are interested in two kinds of specific heats: specific heat at constant volume **cv** and specific heat at constant pressure **cp**.

the specific heat at constant volume cv can be viewed as the energy required to raise the temperature of the unit mass of a substance by one degree as the volume is maintained constant. The energy required to do the same as the pressure is maintained constant **is the specific heat at constant pressure cp.** This is illustrated in Fig. below**.**

For a gas , specific heat depends on whether the gas is at constant pressure or at constant volume.



$$dQ = m\, c_p\, dT$$

$$Q = m\, c_p\, (T_2 - T_1)$$ **specific heat at constant pressure cp.**

$$dQ = m\, c_v\, dT$$

$$Q = m\, c_v\, (T_2 - T_1)$$ **specific heat at constant volume cv.**

For small q & ΔT the ratio q / ΔT tends to limit that indicates the specific heat at a temperature T , thus :

$$c = \lim_{\Delta T \to 0} \frac{q}{\Delta T} = \frac{\delta q}{\delta T}$$

$$c_p = \left(\frac{\delta q}{\delta T}\right)_p = \left(\frac{\delta h}{\delta T}\right)_p$$

$$c_v = \left(\frac{\delta q}{\delta T}\right)_v = \left(\frac{du}{\delta T}\right)_v$$

Where :
δh = change in the enthalpy
δu = change in the internal energy
The unit of the specific heat in the SI units is $\frac{J}{kg\,.k}$

Internal energy (U , u)

Internal energy is defined earlier as the sum of all the microscopic forms of energy of a system. It is related to the molecular structure and the degree of molecular activity and can be viewed as the sum of the kinetic and potential energies of the molecules.

It can be concluded that the net energy transfer to the system in each of these processes must be the same. It follows that heat interactions also involve energy transfer. Denoting the amount of energy transferred to a closed system in heat interactions by Q, these considerations can be summarized by the closed system energy balance:

$$dE = dU + d(\mathrm{KE}) + d(\mathrm{PE}) = \delta Q - \delta W$$

$$(U_2 - U_1) + (KE_2 - KE_1) + (PE_2 - PE_1) = Q - W$$

Assume that there is no change in KE. (The system is steady) ,and there is no change in potential energy (z = 0). Then the above equation become :

$$(U_2 - U_1) = Q - W$$

For must substance , the internal energy, where is no phase change is involved ,depends strongly on temperature and rather weakly on pressure or volume ,and when no external work is done then :

$$\Delta U = (U_2-U_1) = Q = cv\,\Delta T$$

$$Q=m\,cv\,(T_2-T_1)$$

Then : $\Delta U=m\,cv\,(T_2-T_1)$

$$or\ \Delta u=cv\,(T_2-T_1) \text{ per unit mass}$$

The unit of internal energy is (J) ,and for specific internal energy is expressed in (kJ /kg).

Enthalpy:

$$\left(U_2-U_1\right)+\left(KE_2-KE_1\right)+\left(PE_2-PE_1\right)=Q-W$$

Assume that there is no change in KE. (The system is steady) ,and there is no change in potential energy (z = 0). Then the above equation become :

$$\left(U_2-U_1\right)=Q-W$$

and $W=P(V_2-V_1)$

then $Q\text{-}P(V_2\text{-}\ V_1)=(U_2\text{-}U_1)\ \rightarrow\ Q=(U+PV)_1\text{-}\ (U+PV)_2$

$$Q= H_2\text{-}H_1$$

we frequently encounter the combination of properties **(U +Pv).** For the sake of simplicity and convenience, this combination is defined as a new property enthalpy, and given the symbol h for specific enthalpy:

$$h = u + Pv \quad \text{in (kJ /kg)}$$

$$V = mv \, (\text{or } N\bar{v})$$
$$U = mu \, (\text{or } N\bar{u})$$
$$H = mh \, (\text{or } N\bar{h}), \text{ etc.}$$

$$q_{1\text{-}2} = h_2 \text{-} h_1$$

for a constant pressure process the energy equation can be written as :

$$q_{1-2} = \; c_p \; dT \; \rightarrow dh = c_p dT = \int_{T_1}^{T_2} c_p \; dT = \; c_p(T_2 - T_1)$$

Note : enthalpy and internal energy can be found in the steam table.

Perfect gas low

$PV = mRT$

$PV = nR_O T$

Where

m:mass (kg)

n:number of moles

R:specific gas constant (kj/kg.k)

R_O:universal gas constant =8.314 kj/mole .k

$R = \frac{R_O}{\mathcal{M}}$ $\qquad n = \frac{mass}{\mathcal{M}} = \frac{m}{\mathcal{M}}$

$\mathcal{M}$: Molecular weight

Gas
mixture
A + B
V , T
$P_A + P_B$

Molecular weight	
Gases	**μ**
O_2	**32**
N_2	**28**
CO	**28**
C	**12**
CO_2	**44**
H_2O	**18**
H_2	**2**

OTE: 1 mole of air =(0.21 mole of O_2 +0.79 mole of N_2)

1 kg of air =(0.233 kg of O_2 + 0.767 kg of N_2)

Ideal-Gas Mixtures

Two important and useful concepts used to characterize the composition of a mixture are the constituent mole fractions and mass fractions. Consider a multicomponent mixture of gases composed of N_1 moles of species 1, N_2 moles of species 2, etc. The **mole fraction of species *i***, χ_i, is defined as the fraction of the total number of moles in the system that are species i; i.e.,

$$\chi_i \equiv \frac{N_i}{N_1 + N_2 + \ldots N_i + \ldots} = \frac{N_i}{N_{\text{tot}}}. \qquad 3$$

Similarly, the **mass fraction of species *i***, Y_i, is the amount of mass of species i compared with the total mixture mass:

$$Y_i \equiv \frac{m_i}{m_1 + m_2 + \ldots m_i + \ldots} = \frac{m_i}{m_{\text{tot}}}. \qquad 4$$

Note that, by definition, the sum of all the constitutent mole (or mass) fractions must be unity, i.e.,

$$\sum_i \chi_i = 1 \qquad 5$$

$$\sum_i Y_i = 1. \qquad 6$$

Mole fractions and mass fractions are readily converted from one to another using the molecular weights of the species of interest and of the mixture:

$$Y_i = \chi_i MW_i / MW_{\text{mix}} \qquad 7$$

$$\chi_i = Y_i MW_{\text{mix}} / MW_i. \qquad 8$$

The **mixture molecular weight**, $\boldsymbol{MW_{\text{mix}}}$, is easily calculated from a knowledge of either the species mole or mass fractions:

$$MW_{\text{mix}} = \sum_i \chi_i MW_i \qquad 9$$

$$MW_{\text{mix}} = \frac{1}{\sum_i (Y_i / MW_i)}. \qquad 10$$

Species mole fractions are also used to determine corresponding species partial pressures. The **partial pressure of the *i*th species, $\boldsymbol{P_i}$**, is the pressure of the *i*th species if it were isolated from the mixture at the same temperature and volume as the mixture. For ideal gases, the mixture pressure is the sum of the constituent partial pressures:

$$P = \sum_i P_i. \qquad 11$$

The partial pressure can be related to the mixture composition and total pressure as

$$P_i = \chi_i P. \qquad 12$$

For ideal-gas mixtures, many **mass- (or molar-) specific mixture properties** are calculated simply as mass (or mole) fraction weighted sums of the individual species-specific properties. For example, mixture enthalpies are calculated as

$$h_{\text{mix}} = \sum_i Y_i h_i \qquad \text{13a}$$

$$\bar{h}_{\text{mix}} = \sum_i \chi_i \bar{h}_i. \qquad \text{13b}$$

Other frequently used properties that can be treated in this same manner are internal energies, u and $\bar{u}$. Note that, with our ideal-gas assumption, neither the pure-species properties (u_i, $\bar{u}_i$, h_i, $\bar{h}_i$) nor the mixture properties depend on pressure.

The mixture entropy also is calculated as a weighted sum of the constituents:

$$s_{\text{mix}}(T, P) = \sum_i Y_i s_i(T, P_i) \qquad \text{14a}$$

$$\bar{s}_{\text{mix}}(T, P) = \sum_i \chi_i \bar{s}_i(T, P_i). \qquad \text{14b}$$

In this case, however, the pure-species entropies (s_i and $\bar{s}_i$) depend on the species partial pressures as indicated in Eqn. 2.16. The constituent entropies in Eqn. 2.16 can be evaluated from standard-state ($P_{\text{ref}} \equiv P^o = 1$ atm) values as

$$s_i(T, P_i) = s_i(T, P_{\text{ref}}) - R \ln \frac{P_i}{P_{\text{ref}}} \qquad \text{15a}$$

$$\bar{s}_i(T, P) = \bar{s}_i(T, P_{\text{ref}}) = R_u \ln \frac{P_i}{P_{\text{ref}}}. \qquad \text{15b}$$

Standard-state molar specific entropies are tabulated in Appendix A for many species of interest to combustion.

Latent Heat of Vaporization

In many combustion processes, a liquid–vapor phase change is important. For example, a liquid fuel droplet must first vaporize before it can burn; and, if cooled sufficiently, water vapor can condense from combustion products. Formally, we define the **latent heat vaporization, h_{fg}**, as the heat required in a constant-pressure process to completely vaporize a unit mass of liquid at a given temperature, i.e.,

$$h_{fg}(T, P) \equiv h_{\text{vapor}}(T, P) - h_{\text{liquid}}(T, P), \qquad 16$$

where T and P are the corresponding saturation temperature and pressure, respectively. The latent heat of vaporization is also known as the **enthalpy of vaporization**. Latent heats of vaporization for various fuels at their normal (1 atm) boiling points are tabulated in Table B.1 (Appendix B).

The latent heat of vaporization at a given saturation temperature and pressure is frequently used with the **Clausius–Clapeyron equation** to estimate saturation pressure variation with temperature:

Ex1: a rigid tank contains 4 kg of O_2 and 3 kg of N_2 and 5 kg of CO_2 . at press of 2 bar and temperature of 25 ºC . find gravimetric and volumetric analysis .

Sol:

Gases	M_i(kg/kmole)	m_i(kg)	$n_i = m_i / M_i$	$X_i = n_i / \sum n_i$	$Y_i = m_i / \sum m_i$
O_2	32	4	0.125	0.362	0.333
N_2	28	3	0.107	0.310	0.25
CO_2	44	5	0.1136	0.327	0.4166
		$\sum m_i = 12$	$\sum n_i = 0.345$	$\sum X_i = 1$	$\sum Y_i = 1$

Lecture No(2)

FUEL AND COMBUSTION

1. Class: third Year
2. Subject: FUEL AND COMBUSTION
3. Number of weeks: Two week
4. Central idea: Study FUEL AND COMBUSTION
5. The Test:

FUEL AND COMBUSTION

Any material that can be burned to release thermal energy called a **fuel most** familiar fuels consist primarily of hydrogen and carbon. They called hydrocarbon fuel and denoted by general formula C_nH_m .hydrocarbon fuels exist in all phases, some examples

Hydrocarbon fuel
- Solid (coal)
- Liquid (petrol)
- Gas (methane)

Combustion

Combustion may by defined as a rapid chemical reaction between fuel and air (oxygen) it's usually accompanied by aflame and heat is released during this reaction.

Combustion may by classified as follows :

1-stoichiometric combustion

2-incomplete combustion

3-complete combustion

1-stoichiometric combustion :this type of combustion occurs when the amount of oxygen (air) available is just enough to convert all carbon to carbon dioxide CO_2 and all hydrogen to water H_2O with no oxygen left over (CO_2 , H_2O, N_2)

$$\underbrace{\underset{fuel}{CnH_m} + \underset{Air}{A}(0.21O_2 + 0.79N_2)}_{\text{Reactance}} \longrightarrow \underbrace{CO_2 + H_2O + N_2}_{\text{products}}$$

$$A = n + \frac{m}{4}$$

$$CH_4 + A\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow CO_2 + 2H_2O + 2 * \frac{79}{21}N_2$$

$$A = 1 + \frac{4}{4} = 2$$

$$CH_4 + 2\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow CO_2 + 2H_2O + 2 * \frac{79}{21}N_2$$

2-incomplete combustion : this type of combustion occurs when the amount of oxygen (Air) is not enough to convert all carbon to CO_2, hence a carbon monoxide CO will be present in the products (CO_2 ,CO, H_2O, N_2)

$$CH_4 + 1.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow aCO_2 + bCO + 2H_2O + 1.5 * \frac{79}{21}N_2$$

3-complete combustion : this type of combustion occurs when the amount of O_2 (air) is more than enough to convert all carbon and hydrogen to CO_2 and H_2O .hence a certain amount of O_2 will be in the products (CO_2 ,O_2, H_2O, N_2)

$$CH_4 + 2.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow CO_2 + aO_2 + 2H_2O + 2.5 * \frac{79}{21}N_2$$

Definition

Air fuel ratio *(A/F)* :it is the ratio between mass of air to mass of fuel

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} \qquad m = n.\mathcal{M}$$

Ex1: $CH_4 + 2\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow CO_2 + 2H_2O + 2 * \frac{79}{21}N_2$

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{2*32+2*3.76*28}{[(1*12)+(4*1)]} = 17.16$$

- $\%excess\ of\ air = \frac{(A/F)_{actual} - (A/F)_{stoich}}{(A/F)_{stoich}} * 100$
- $\%\ theoretical\ of\ air = \frac{(A/F)_{actual}}{(A/F)_{stoich}} * 100$
- Equivalence ratio (mixture strength) *(M.S)* :it is the ratio between stoichiometric *(A/F)* to actual *(A/F)*

  $$\phi = M.S = \frac{(A/F)_{stoich}}{(A/F)_{actual}}$$

  $$If\ \phi > 1 \Rightarrow Incomplete\ combustion(rich\ fuel\ mixtures)\ (CO_2 + CO + H_2O + N_2)$$

  $$If\ \phi < 1 \Rightarrow complete\ combustion(lean\ or\ poor\ or\ weak\ \ fuel\ mixtures)\ (CO_2 + O_2 + H_2O + N_2)$$

  $$If\ \phi = 1 \Rightarrow stoichiometric\ combustion\ (CO_2 + H_2O + N_2)$$

  Ex2: A hydrocarbon fuel C_4H_{10} is burned with the following cases :

  1- 125% theoretical of air.
  2- 80% theoretical of air.
  3- With ϕ =0.85.

Write the equation of combustion and Find the *(A/F)* for each case

Sol:

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1- $C_4H_{10} + 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + 5H_2O + 6.5 * \frac{79}{21}N_2$

$A = n + \frac{m}{4}$ =4+10/4=6.5

ثانيا كتابة معادلة الاحتراق الحقيقة

$$C_4H_{10} + 1.25 * 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + 5H_2O + aO_2 + 1.25 * 6.5 * \frac{79}{21}N_2$$

Oxygen balance

1.25*6.5*2=4*2+5+2a

a= 1.625

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{1.25 * 6.5 * 32 + 1.25 * 6.5 * \frac{79}{21} * 28}{[(4 * 12) + (10 * 1)]} = 19.23$$

2- $C_4H_{10} + 0.8 * 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow aCO_2 + bCO + dH_2O + 0.8 * 6.5 * \frac{79}{21}N_2$

Carbon balance

4=a+b a=4-b ….(1)

Hydrogen balance 10=2d d=5

Oxygen balance 0.8*6.5*2=2a+b+d

10.4=2(4-b)+b+5 b=2.6 a=1.4

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{0.8 * 6.5 * 32 + 0.8 * 6.5 * \frac{79}{21} * 28}{[(4 * 12) + (10 * 1)]} = 12.12$$

3-$C_4H_{10} + \frac{6.5}{0.85}\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + aO_2 + 5H_2O + \frac{6.5}{0.85} * \frac{79}{21}N_2$

Oxygen balance

(6.5/0.85)* 2 =4*2+2a+5 a=1.147

$$\frac{A}{F}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{\left(\frac{6.5}{0.85}\right)*32+\left(\frac{6.5}{0.85}\right)*\frac{79}{21}*28}{[(4*12)+(10*1)]}=18.10$$

Ex3: A hydrocarbon fuel C_3H_8 is burned with the following cases:

1-10% less of air.

2-20% excess of air.

Write the equation of combustion and Find

a-the *(A/F)* for each case.

b-the equivalence ratio.

Sol: stoich equation

$$1\text{- } C_3H_8+5\left(O_2+\frac{79}{21}N_2\right)\longrightarrow 3CO_2+4H_2O+5*\frac{79}{21}N_2$$

$$\left(\frac{A}{F}\right)_{stoic}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{5*32+5*\frac{79}{21}*28}{[(3*12)+(8*1)]}=15.6$$

Actual combustion equation

$$C_3H_8+0.9*5\left(O_2+\frac{79}{21}N_2\right)\longrightarrow aCO_2+bCO+dH_2O+0.9*5*\frac{79}{21}N_2$$

Carbon balance

3=a+b   a=3-b ….(1)

Hydrogen balance 8=2d   d=4

Oxygen balance 0.9*5*2=2a+b+d

9=2(3-b)+b+4   b=1   a=2

$$\left(\frac{A}{F}\right)_{actual}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{0.9*5*32+0.9*5*\frac{79}{21}*28}{[(3*12)+(8*1)]}=14.045$$

$$\phi=M.S=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{15.6}{14.045}=1.11>1\ incomplete\ combustion$$

2- 20% excess of air.

Actual combustion equation

$$C_3H_8+1.2*5\left(O_2+\frac{79}{21}N_2\right)\longrightarrow 3CO_2+aO_2+4H_2O+1.2*5*\frac{79}{21}N_2$$

Oxygen balance 1.2*5*2=3*2+2a+4

a=1

$$\left(\frac{A}{F}\right)_{actual}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{1.2*5*32+1.2*5*\frac{79}{21}*28}{[(3*12)+(8*1)]}=18.727$$

$$\phi=M.S=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{15.6}{18.727}=0.833<1\ complete\ combustion$$

Ex4:Ethanol $CH_3CH_2OH\ \ or\ \ C_2H_5OH\quad C_nH_mO_wH$

Stoichiometric equation

$$CH_3CH_2OH+A(O_2+3.76N_2)\longrightarrow aCO_2+bH_2O+f3.76N_2$$

$$A=n+\frac{m}{4}-\frac{w}{2}=2+\frac{6}{4}-\frac{1}{2}=3$$

$$CH_3CH_2OH+3(O_2+3.76N_2)\longrightarrow 2CO_2+3H_2O+3*3.76N_2$$

$$\frac{A}{F}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{3*(32+3.76*28)}{[(2*12)+(6*1)+(16*1)]}=8.953$$

$$\phi=\frac{(A/F)_{stoich}}{(A/F)_{actual}}$$

$$for\ \phi=0.6=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{8.953}{(A/F)_{actual}}$$

$$\boldsymbol{(A/F)_{actual}=14.921}$$

$$for\ \phi=0.8=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{8.953}{(A/F)_{actual}}$$

$$\boldsymbol{(A/F)_{actual}=11.19125}$$

$$for\ \phi=1=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{8.953}{(A/F)_{actual}}$$

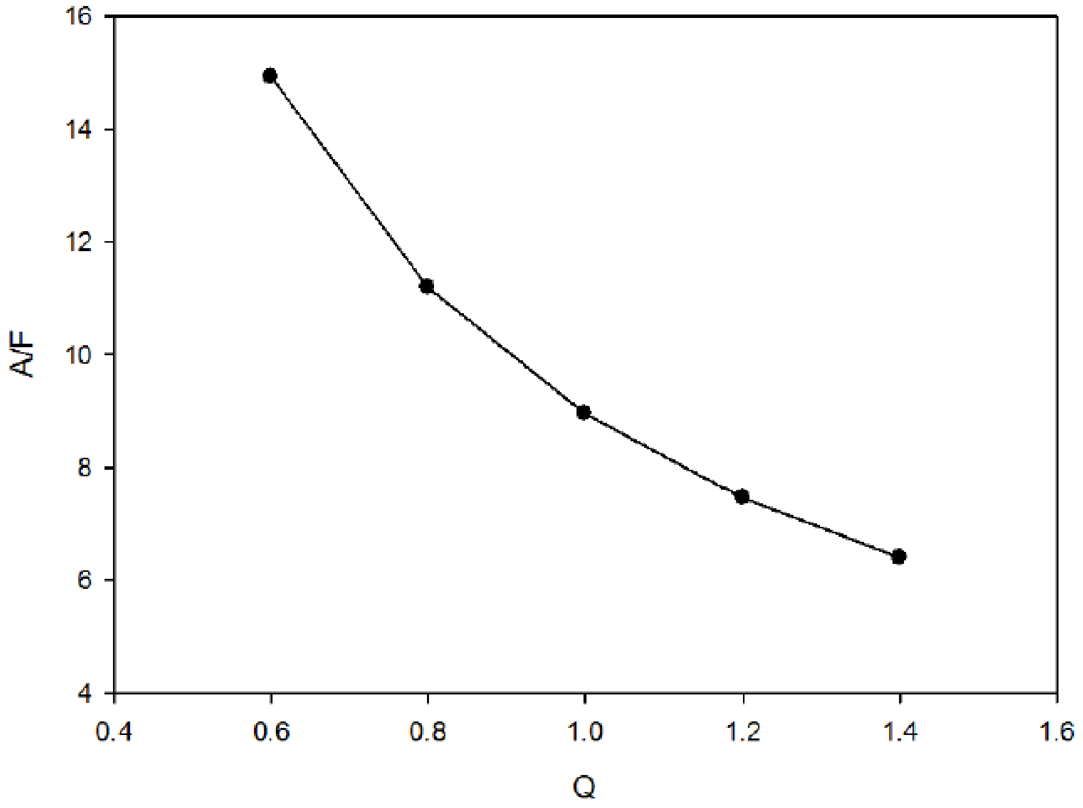
$$\boldsymbol{(A/F)_{actual}=8.953}$$

$$for\ \phi=1.2=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{8.953}{(A/F)_{actual}}$$

$$\boldsymbol{(A/F)_{actual}=7.4608}$$

$$for\ \phi=1.4=\frac{(A/F)_{stoich}}{(A/F)_{actual}}=\frac{8.953}{(A/F)_{actual}}$$

$$\boldsymbol{(A/F)_{actual}=6.395}$$



Effect of Equivalence ratio on Air fuel ratio (A/F)

Ex5:A spark ignition engine uses a hydrocarbon fuel gasoline C_8H_{15} .the engine running of mixture strength of 1.2 . determine

1) The air -fuel ratio
2) The wet and dry volumetric exhaust analysis .
3) The wet and dry gravimetric exhaust analysis .

Sol:

Sol: أول خطوة هي كتابة معادلة الاحتراق المثالية

1- $C_8H_{15} + A(O_2 + 3.76N_2) \longrightarrow 8CO_2 + 7.5H_2O + A * \frac{79}{21}N_2$

$A = n + \frac{m}{4}$ =8+15/4=

$$C_8H_{15} + 11.75(O_2 + 3.76N_2) \longrightarrow 8CO_2 + 7.5H_2O + 11.75 * \frac{79}{21}N_2$$

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{11.75 * 32 + 11.75 * 3.76 * 28}{[(8 * 12) + (15 * 1)]} = 14.53$$

$$M.S = \phi = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = 1.2 = \frac{14.53}{(A/F)_{actual}} \rightarrow (A/F)_{actual} = 12.109$$

ثانيا كتابة معادلة الاحتراق الحقيقة

$$C_8H_{15} + \frac{11.75}{1.2}\left(O_2 + \frac{79}{21}N_2\right)$$
$$\longrightarrow aCO_2 + bCO + dH_2O + \frac{11.75}{1.2} * 3.76 * N_2$$

Carbon balance

3=a+b   a=8-b ….(1)

Hydrogen balance 15=2d   d=7.5

Oxygen balance 9.79*2=2a+b+d

19.58=2(8-b)+b+5   b=3.92   a=4.08

$$\frac{A}{F}=\frac{mass\ of\ air}{mass\ of\ fuel}=\frac{\frac{11.75}{1.2}*32+\frac{11.75}{1.2}*3.76*28}{[(8*12)+(15*1)]}=12.109$$

Product	*Mi*(kg/kmole)	ni	Xi=ni/∑ni (wet)	Xi=ni/∑ni(dry)	mi=ni* *Mi*	Yi=mi/∑mi(wet)	Yi=mi/∑mi(dry)
CO_2	44	4.08	0.078	0.091	179.52	0.1234	0.136
CO	28	3.92	0.074	0.087	109.76	0.075	0.0825
H_2O	18	7.5	0.143	**With out H2o**	135	0.0928	
N_2	28	36.81	0.703	0.821	1030	0.708	0.7803
		∑ni=52.3	∑Xi=1	∑Xi=1	∑mi=1454.2	∑Yi=1	∑Yi=1

Engine exhaust analysis

The control system of modern (smart automobile engine) includes (sensors) that continuously monitor for the exhaust leaving the engine These sensors determine the chemical composition of the hot exhaust by various (chemical , electronic and thermal methods)

Ex6: 4-cylinder engine ($\mathbf{C_3H_8}$ fuel) a dry analysis of the engine exhaust of the following volumetric percentage CO2 4.9% , CO 9.79% , O2 2.45% Calculate ϕ

Sol:

For dry engine product =4.9+9.79+2.45 = 17.14 % and that remaining gas (N2) =82.86% if unknow of fuel burned with an unknown amount of air , the resulting reaction is

stoich equation

$$C_3H_8 + 5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 3CO_2 + 4H_2O + 5 * \frac{79}{21}N_2$$

$$\left(\frac{A}{F}\right)_{stoic} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{5 * 32 + 5 * \frac{79}{21} * 28}{[(3 * 12) + (8 * 1)]} = 15.6$$

Actual combustion equation

$$xC_3H_8 + y(O_2 + 3.76N_2) \longrightarrow 4.9CO_2 + 9.79CO + ZH_2O + 2.45O_2 + 82.86N_2$$

z -no of H2O vapor removed before dry analysis

N2 : y * 3.76 = 82.86 » y =22.037

C : 3*x =4.9 +9.79 » x =4.9

H : 8*x=8(4.9)=2*Z » Z =19.588

$$4.9C_3H_8 + 22.037(O_2 + 3.76N_2) \longrightarrow 4.9CO_2 + 9.79CO + 19.588H_2O + 2.45O_2 + 82.86N_2$$

÷ 4.9

$$C_3H_8 + 4.5(O_2 + 3.76N_2) \longrightarrow CO_2 + 2\,CO + 4H_2O + 0.5O_2 + 16.92\,N_2$$

$$\left(\frac{A}{F}\right)_{act} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{4.5 * 32 + 4.5 * 3.76 * 28}{[(3 * 12) + (8 * 1)]} = 14.12$$

$$\phi = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{15.89}{14.12} = 1.11$$

H.W:

4-cylinder engine (**C_8H_{18}** fuel) a dry analysis of the engine exhaust of the following volumetric percentage CO2 9.85% , CO 0.9% , O2 5.7% Calculate ϕ

Lecture No (4)

Application of 1st law of thermodynamic on combustion process

1. Class: third Year

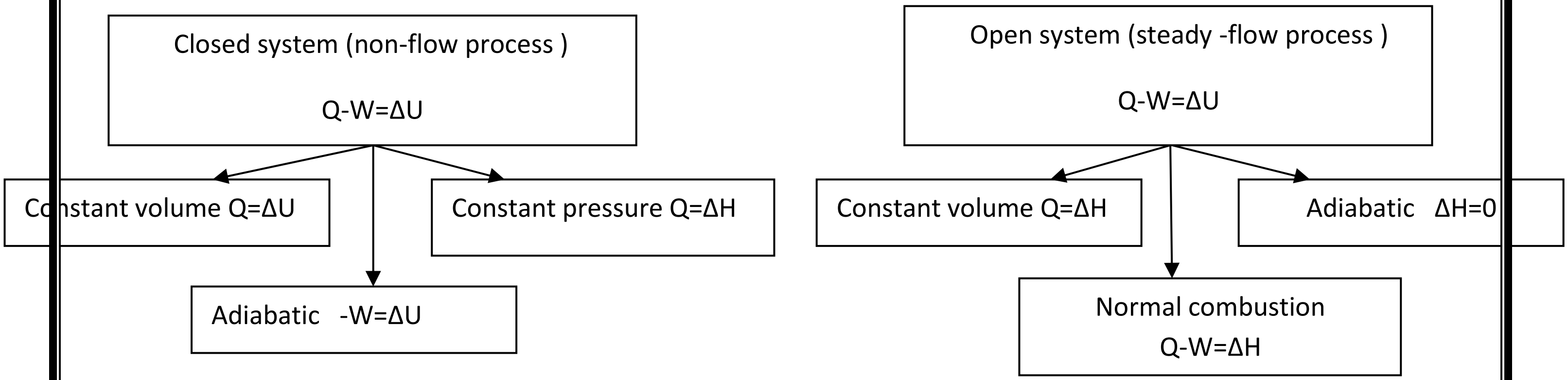
2. Subject Application of 1st law of thermodynamic on combustion process

3. Number of weeks: Two week

4. Central idea: Study Application of 1st law of thermodynamic on combustion process

5. The Test:

Application of 1st law of thermodynamic on combustion process



$$Q = \Delta H$$

$$Q = \sum_P n_i h_i - \sum_R n_i h_i$$

$$h_i = \left(h_{f^o} + \Delta h\right)$$

h_i: enthalpy of each an item

h_{f^o}: enthalpy of formation @(298 k)

$$\Delta h = h(T) - h_{f^o}(298)$$

or

$$Q = \Delta U$$

$$h = u + Pv \quad \rightarrow u = h - pv$$

$$Pv = n\, R_u\, T$$

$$u = h - n\, R_u\, T$$

$$U_{reac} = \sum_R n_i h_{reac} - \sum_R n\,_i R_u\, T_i$$

$$U_{prod} = \sum_P n_i h_{reac} - \sum_P n\,_i R_u\, T_i$$

$$Q = \Delta U = U_{prod} - U_{reac}$$

$$= \left(\sum_P n_i h_{reac} - \sum_P n\,_i R_u\, T_i\right) - (\sum_R n_i h_{reac} - \sum_R n\,_i R_u\, T_i\,)$$

Ex: An I.E C_3H_8 (0.00005 kg) in each cylinder during cycle $\eta_{comb} = 0.95$

Combustion start T=700K & p=2000 Kpa the end of compression is Texh 1200 K calculate and $for\ \phi = 0.8$ calculate Combustion heat

Sol:

Stoichiometric equation

$$C_3H_8 + A(O_2 + 3.76N_2) \longrightarrow aCO_2 + bH_2O + A * 3.76N_2$$

$$A = n + \frac{m}{4} = 3 + \frac{8}{4} = 5$$

$$C_3H_8 + 5(O_2 + 3.76N_2) \longrightarrow 3CO_2 + 4H_2O + 5 * 3.76N_2$$

$$for\ \phi = 0.8$$

$$C_3H_8 + \frac{5}{0.8}(O_2 + 3.76N_2) \longrightarrow aCO_2 + bH_2O + wO_2 + 5 * 3.76N_2$$

$$C_3H_8 + \frac{5}{0.8}(O_2 + 3.76N_2) \longrightarrow 3CO_2 + 4H_2O + 1.25O_2 + 6.25 * 3.76N_2$$

$$Q = \Delta H$$

$$Q = \sum_{P} n_i h_i - \sum_{R} n_i h_i$$

$$h_i = \left(h_{f^o} + \Delta h\right)$$

At T=700K before combustion using data from Appendix **A** and table B1 & B2

نحسب الانثالبي للوقود من خلال المعادله والجدول الاتي عند 700k

وبقيه قيم الانثالبي للمتقاعلات من الجدول A

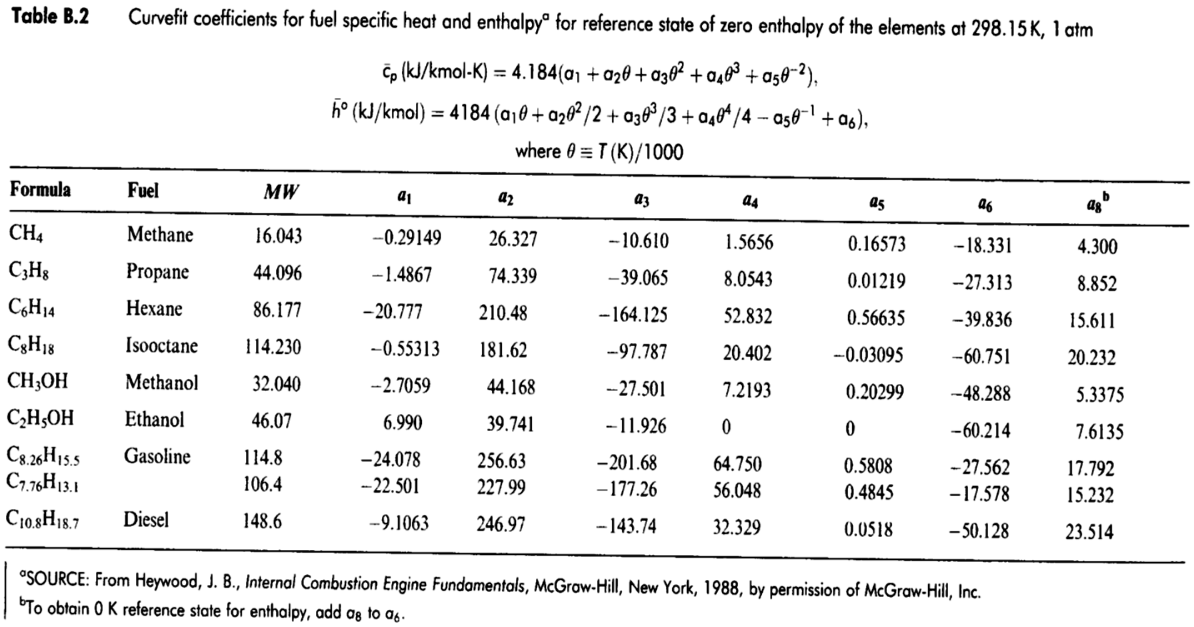


Table B.2 Curvefit coefficients for fuel specific heat and enthalpy[a] for reference state of zero enthalpy of the elements at 298.15 K, 1 atm

$$\bar{c}_p\ (\text{kJ/kmol-K}) = 4.184(a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2}),$$

$$\bar{h}^o\ (\text{kJ/kmol}) = 4184\,(a_1\theta + a_2\theta^2/2 + a_3\theta^3/3 + a_4\theta^4/4 - a_5\theta^{-1} + a_6),$$

$$\text{where } \theta \equiv T\,(\text{K})/1000$$

Formula	**Fuel**	***MW***	a_1	a_2	a_3	a_4	a_5	a_6	a_8[b]
CH_4	Methane	16.043	−0.29149	26.327	−10.610	1.5656	0.16573	−18.331	4.300
C_3H_8	Propane	44.096	−1.4867	74.339	−39.065	8.0543	0.01219	−27.313	8.852
C_6H_{14}	Hexane	86.177	−20.777	210.48	−164.125	52.832	0.56635	−39.836	15.611
C_8H_{18}	Isooctane	114.230	−0.55313	181.62	−97.787	20.402	−0.03095	−60.751	20.232
CH_3OH	Methanol	32.040	−2.7059	44.168	−27.501	7.2193	0.20299	−48.288	5.3375
C_2H_5OH	Ethanol	46.07	6.990	39.741	−11.926	0	0	−60.214	7.6135
$C_{8.26}H_{15.5}$	Gasoline	114.8	−24.078	256.63	−201.68	64.750	0.5808	−27.562	17.792
$C_{7.76}H_{13.1}$		106.4	−22.501	227.99	−177.26	56.048	0.4845	−17.578	15.232
$C_{10.8}H_{18.7}$	Diesel	148.6	−9.1063	246.97	−143.74	32.329	0.0518	−50.128	23.514

[a] SOURCE: From Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, by permission of McGraw-Hill, Inc.

[b] To obtain 0 K reference state for enthalpy, add a_8 to a_6.

$$H_{rac} = 1(-103847 + 44792) + 6.25\,(0 + 12503) + 6.25 * 3.76(0 + 11942) = 299725\text{Kj/KMole}$$

Enthalpy of product at Texh=1200k

$$H_{prod} = 3(-393{,}546 + 44488) + 4\,(-241{,}845 + 34518) + 6.25 * 3.76(0 + 28118) + 1.25(0 + 29775) = -1302758\text{ Kj/KMole}$$

$$Mw\ of\ C_3H_8 = 36 + 8 = 44\ kg/kmol$$

$$Q = \sum_P n_i h_i - \sum_R n_i h_i$$

$$Q = \left(\frac{-1302758 - 299725}{44}\right) * 0.0005 = -1.821\text{ Kj}$$

الاشاره السالبه معناها ان الاتفاعل باعث للحراره و اذا الاشاره موجبه فالتفاعل ماص للحراره

Ex: determine HHV & LHV at 298k of gases n-decane $C_{10}H_{22}$ per kmol of fuel & per kg of fuel (Mw=142.284 kg/kmol) if $\boldsymbol{h_{fg}}$ of n-decane (359 kj/kg)

At 298 k , what are the HHV & LHV of liquid n- decane

Sol:

$$C_{10}H_{22} + A(O_2 + 3.76N_2) \longrightarrow 10CO_2 + 11H_2O + A * 3.76N_2$$

$$A = n + \frac{m}{4} = 10 + \frac{22}{4} = 15.5$$

$$C_{10}H_{22} + 15.5(O_2 + 3.76N_2) \longrightarrow 10CO_2 + 11H_2O + 15.5 * 3.76N_2$$

$$Q = \Delta H = H_{prod} - H_{reac} = \sum_P n_i h_i - \sum_R n_i h_i$$

$$h_i = \left(h_{f^o} + \Delta h\right)$$

HHV عندما يكون الماء في النواتج بهيئه سائل

$h_{fg} = h_g - h_l$

$h_{l(h2o)} = h_{g(h2o)} - h_{fg} = \mathbf{-241,845 - 440,10 = -285,857}\,\frac{kJ}{kmol}$

$H_{reac} = \sum_R n_i h_i = \sum_R n_i\left(h_{f^o} + \Delta h\right) = -249{,}659 + 15.5(0+0) + 15.5 * 3.76(0+0) = -249{,}659\,\frac{kJ}{kmol}$

$H_{prod} = \sum_p n_i h_i = \sum_p n_i\left(h_{f^o} + \Delta h\right) = 10(-393{,}546) + 11(\mathbf{-285,857}) + 15.5 * 3.76(0+0) = -7{,}079{,}887\,\frac{kJ}{kmol}$

$$Q = \Delta H = H_{prod} - H_{reac} = -7{,}079{,}887 - (-249659)$$
$$= 6{,}830{,}096\,\frac{kJ}{kmol}$$

لايجاد قيمه ΔH لكغم من الوقود نقسم على الوزن الجزئي

$$\Delta H = \frac{\Delta H}{Mw} = \frac{6{,}830{,}096}{142.284} = 48{,}000\,\frac{kJ}{kg}$$

For the LHV $h_{g(h2o)} = = \mathbf{-241,845}$

$H_{prod} = \sum_p n_i h_i = \sum_p n_i\left(h_{f^o} + \Delta h\right) = 10(-393{,}546) + 11(\mathbf{-241,845}) + 15.5 * 3.76(0+0) = -6{,}595{,}755\,\frac{kJ}{kmol}$

$$Q = \Delta H = H_{prod} - H_{reac} = -6{,}595{,}755 - (-249659)$$
$$= 6{,}345{,}986\,\frac{kJ}{kmol}$$

لايجاد قيمه ΔH لكغم من الوقود نقسم على الوزن الجزئي

$$\Delta H = \frac{\Delta H}{Mw} = \frac{6{,}345{,}986}{142.284} = 44{,}601\,\frac{kJ}{kg}$$

B)

If $\boldsymbol{h_{fg}}$ (fuel)= 359 kJ/kg of $(C_{10}H_{22})$

H_{reac} = 1=$h_{g(C_{10}H_{22})} - h_{fg}$ =

$$H.H.V = \Delta hc(\boldsymbol{liquid}) = \mathbf{48004 - 359 = 47645}\,\frac{kJ}{kg\text{ of }(C_{10}H_{22})}$$

$$L.H.V = \Delta h\boldsymbol{c}(\boldsymbol{gas}) = \mathbf{44602 - 359 = 44243}\,\frac{kJ}{kg\text{ of }(C_{10}H_{22})}$$

ملاحظه مهمه : اذا طلب الناتج لوحده كتله للخليط (kJ/kg per of mixture)

$$\Delta h_C\left(\frac{kJ}{kg\ mix}\right) = \Delta h_C\left(\frac{kJ}{kg\ fuel}\right).\frac{\dot m_{fuel}}{\dot m_{mix}}$$

$$\frac{\dot m_{fuel}}{\dot m_{mix}} = \frac{\dot m_{fuel}}{\dot m_{fuel}+\dot m_{air}} = \frac{1}{1+(A/F)}$$

$$\Delta h_C\left(\frac{kJ}{kg\ mix}\right) = \Delta h_C\left(\frac{kJ}{kg\ fuel}\right).\frac{1}{1+(A/F)}$$

Ex2: A mixture of C_4H_{10} and air of strength 1.25 is initially at 298K and 1 bar in a piston cylinder arrangement where is loaded by a weigh .If the combustion occurs and the temperature is 600k , calculate Combustion heat

Sol:

اول خطوة كتابة معادلة الاحتراق المثالية

$$C_4H_{10} + 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + 5H_2O + 6.5 * \frac{79}{21}N_2$$

ثانيا كتابة معادلة الاحتراق الحقيقة

$$C_4H_{10}+\frac{6.5}{1.25}\left(O_2+\frac{79}{21}N_2\right)\longrightarrow aCO_2+bCO+5H_2O+\frac{6.5}{1.25}*\frac{79}{21}N_2$$

Carbon balance

4=a+b a=4-b ….(1)

Oxygen balance 6.5/1.25*2=2a+b+5

10.4=2(4-b)+b+5 b=2.6 a=1.4

Constant pressure + closed system Q=ΔH

$$Q=\Delta H$$

$$Q=\sum_{P}n_ih_i-\sum_{R}n_ih_i$$

$$h_i=\left(h_{f^o}+\Delta h\right)$$

ملاحظه : في حاله درجه حراره المتفاعلات (25ºC) او (298K) فان ***hi=hf***

للوقود والانثالبي للعناصر الحره يكون صفر

$$h_i=\left(h_{f^o}+\Delta h\right)$$

h_{f^o} *B1* *من جدول الوقود*

$$\Delta h=h(T)-h(298)$$

T =298 K

$$\Delta h=h(298)-h(298)=0$$

$$h_i=\left(h_{f^o}+\Delta h\right)=\left(h_{f^o}+0\right)=h_{f^o}=-124733\ kJ/k\ mol$$

$$H_{rac} = 1(-124733\,) + \frac{6.5}{1.25}\,(0+0) + \frac{6.5}{1.25} * 3.76(0+0)$$
$$= -124733\text{Kj/Mole}$$

Enthalpy of product at Texh=600k

$$H_{prod} = 1.4(-393549 + 12899) + \;2.6\,(-110541 + 8955)$$
$$+ 5(-241845 + 10528) + \frac{6.5}{1.25} * 3.76(0 + 8905)$$
$$= -1779508\text{ Kj/Mole}$$

$$Mw\ of\ C_4H_{10} = 36 + 8 = 58\ kg/kmol$$

$$Q = \sum_P n_i h_i - \sum_R n_i h_i$$

$$Q = (\frac{-1779508-(-124733)}{58}) = -28530\text{ kJ/kg of }(C_4H_{10})$$

H.W : An I.E C_8H_{16} (0.000055 kg) in each cylinder during cycle $\eta_{comb} = 0.95$

Combustion start T=700K & p=2000 Kpa the end of compression is Texh 1300 K calculate Combustion heat

Lecture No (4)

Adiabatic flame temperature

1. Class: third Year
2. Subject: Adiabatic flame temperature
3. Number of weeks: Two week
4. Central idea: Study Adiabatic flame temperature
5. The Test:

Adiabatic flame temperatures (***Tad***): is ideal theoretical maximum temperature can be obtained for a given fuel and air mixture.

We define two adiabatic flame temperatures: one for constant-pressure combustion and one for constant-volume. If a fuel–air mixture burns adiabatically at constant pressure, the absolute enthalpy of the reactants at the initial state (say, $T = 298\,\mathrm{K}$, $P = 1\,\mathrm{atm}$) equals the absolute enthalpy of the products at the final state ($T = T_{ad}$, $P = 1\,\mathrm{atm}$),

$$H_{\mathrm{reac}}(T_i, P) = H_{\mathrm{prod}}(T_{ad}, P),$$

or, equivalently, on a per-mass-of-mixture basis,

$$h_{\mathrm{reac}}(T_i, P) = h_{\mathrm{prod}}(T_{ad}, P).$$

This first-law statement, Eqn. 2.40, defines what is called the **constant-pressure adiabatic flame temperature**. This definition is illustrated graphically in Fig. 1 Conceptually, the adiabatic flame temperature is simple; however, evaluating this quantity requires knowledge of the composition of the combustion products. At typical flame temperatures, the products dissociate and the

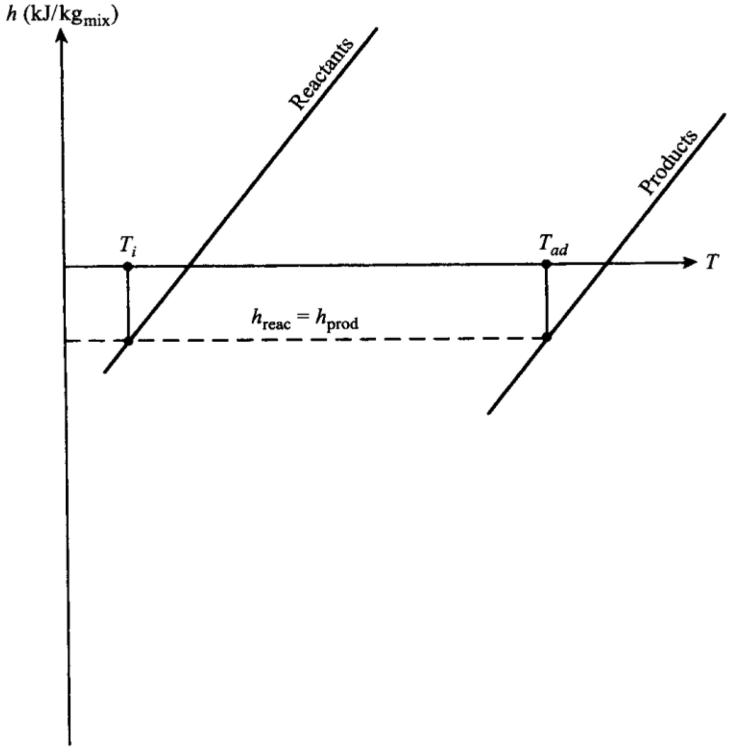


Figure 1 Illustration of constant-pressure adiabatic flame temperature on h–T coordinates.

mixture comprises many species. As shown in Table 2.1 and Table B.1 in Appendix B, flame temperatures are typically several thousand kelvins. Calculating the complex composition by invoking chemical equilibrium is the subject of the next section. The following example illustrates the fundamental concept of constant-pressure adiabatic flame temperatures, while making crude assumptions regarding the product mixture composition and evaluation of the product mixture enthalpy.

Ex1:Find ***Tad*** of C_8H_{18} burned with $\phi = 0.833$ can assumed that the reactants at 700 k after compression stroke

Sol:

Stoichiometric equation

$$C_8H_{18} + A(O_2 + 3.76N_2) \longrightarrow aCO_2 + bH_2O + A * 3.76N_2$$

$$A = n + \frac{m}{4} = 8 + \frac{18}{4} = 5$$

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

$$for\ \phi = 0.833$$

$$C_8H_{18} + \frac{12.5}{0.833}(O_2 + 3.76N_2) \longrightarrow 8CO_2 + 9H_2O + 2.5O_2 + 15 * 3.76N_2$$

To calculate Tad @ Treac=700K

$$0 = \sum_P n_i h_i - \sum_R n_i h_i$$

$$\sum_{Prod} n_i(h_{f^0} + \Delta\text{h})_i = \sum_{Reca} n_i(h_{f^0} + \Delta\text{h})_i$$

$$8(-393546+\Delta \mathrm{h}_{CO_2}) + 9(-241845+\Delta \mathrm{h}_{H_2O}) + 2.5(0+\Delta \mathrm{h}_{O_2}) + 15 * 3.76(0+\Delta \mathrm{h}_{N_2}) = 1(-259280+73473) + 15(0+12499) + 15 * 3.76(0+11937)$$

$$8\Delta \mathrm{h}_{CO_2} + 9\Delta \mathrm{h}_{H_2O} + 2.5\Delta \mathrm{h}_{O_2} + 56.4\Delta \mathrm{h}_{N_2} = 5{,}999{,}535$$

By trial and error find Tad , try T=2400 K

$$8(115{,}779)_{CO_2} + 9(93{,}741)_{H_2O} + 2.5(74{,}453)_{O_2} + 56.4(70{,}640)_{N_2} = 5{,}940{,}130$$

This is too low , so try T=2600 K

$$8(128{,}074)_{CO_2} + 9(104{,}520)_{H_2O} + 2.5(82{,}453)_{O_2} + 56.4(77{,}963)_{N_2} = 6{,}567{,}948$$

This is too high , so ***Tad*** is found by interpolation

Tad* 2419 *K

Ex2: Ethanol $CH_3CH_2OH \quad or \quad C_2H_5OH \quad C_nH_mO_wH$

Stoichiometric equation

$$CH_3CH_2OH + A(O_2 + 3.76N_2) \longrightarrow aCO_2 + bH_2O + f3.76N_2$$

$$A = n + \frac{m}{4} - \frac{w}{2} = 2 + \frac{6}{4} - \frac{1}{2} = 3$$

$$CH_3CH_2OH + 3(O_2 + 3.76N_2) \longrightarrow 2CO_2 + 3H_2O + 3 * 3.76N_2$$

$$\frac{A}{F} = \frac{mass\ of\ air}{mass\ of\ fuel} = \frac{3 * (32 + 3.76 * 28)}{[(2 * 12) + (6 * 1) + (16 * 1)]} = 8.953$$

$$\phi = \frac{(A/F)_{stoich}}{(A/F)_{actual}}$$

$$for\ \phi = 0.6 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

$$\left(\boldsymbol{\frac{A}{F}}\right)_{\boldsymbol{actual}} = \mathbf{14.921}$$

$$for\ \phi = 0.6 \Longrightarrow T_{ad} = 1883.30\ K$$

$$for\ \phi = 0.8 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

$$\left(\boldsymbol{\frac{A}{F}}\right)_{\boldsymbol{actual}} = \mathbf{11.19125}$$

$$for\ \phi = 0.8 \Longrightarrow T_{ad} = 2220.64\ K$$

$$for\ \phi = 1 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

$$(\boldsymbol{A/F})_{\boldsymbol{actual}} = \mathbf{8.953}$$

$$for\ \phi = 1 \Longrightarrow T_{ad} = 2402.64\ K$$

$$for\ \phi = 1.2 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

$$(\boldsymbol{A/F})_{\boldsymbol{actual}} = \mathbf{7.4608}$$

$$for\ \phi = 1.2 \Longrightarrow T_{ad} = 2421.41\ K$$

$$for\ \phi = 1.4 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

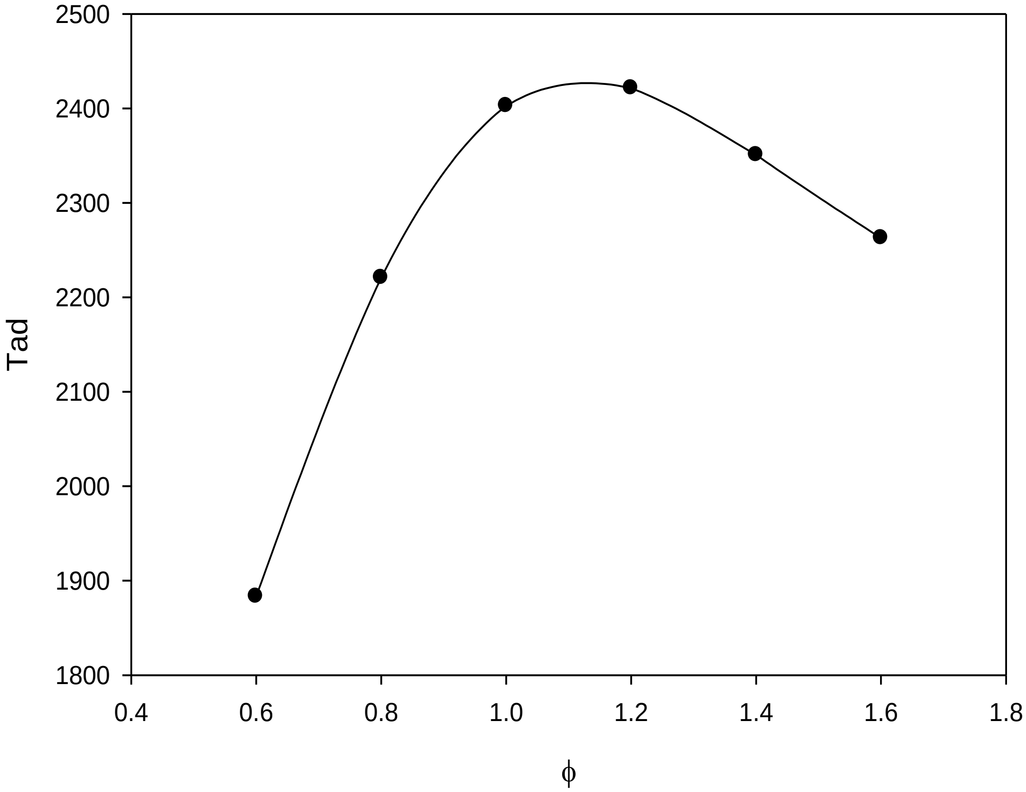
$$(\boldsymbol{A/F})_{\boldsymbol{actual}} = \mathbf{6.395}$$

$$for\ \phi = 1.4 \Longrightarrow T_{ad} = 2350.74\ K$$

$$for\ \phi = 1.6 = \frac{(A/F)_{stoich}}{(A/F)_{actual}} = \frac{8.953}{(A/F)_{actual}}$$

$$\boldsymbol{(A/F)_{actual} = 5.595}$$

$$for\ \phi = 1.4 \Longrightarrow T_{ad} = 2262.85\ K$$



effect of ϕ on Tad at constant pressure

Ex3: Determine adiabatic flame temperature for constant pressure combustion for n-butane burned with 80% theoretical of air can assumed that the reactants at 298 k

Sol:

$$C_4H_{10} + 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow 4CO_2 + 5H_2O + 6.5 * \frac{79}{21}N_2$$

$A = n + \frac{m}{4}$ =4+10/4=6.5

$$C_4H_{10} + 0.8 * 6.5\left(O_2 + \frac{79}{21}N_2\right) \longrightarrow aCO_2 + bCO + dH_2O + 0.8 * 6.5 * \frac{79}{21}N_2$$

Carbon balance

4=a+b   a=4-b ….(1)

Hydrogen balance 10=2d   d=5

Oxygen balance 0.8*6.5*2=2a+b+d

10.4=2(4-b)+b+5   b=2.6   a=1.4

To calculate Tad @ Treac=290K

$$0 = \sum_{P} n_i h_i - \sum_{R} n_i h_i$$

$$\sum_{Prod} n_i(h_{f^o} + \Delta \mathrm{h})_i = \sum_{Reca} n_i(h_{f^o} + \Delta \mathrm{h})_i$$

$$\begin{aligned} 1.4(-393546 + \Delta \mathrm{h}_{CO_2}) + 2.6(-110541 + \Delta \mathrm{h}_{co}) + 5(-241845 \\ + \Delta \mathrm{h}_{H_2O}) + 5.2 * 3.76(0 + \Delta \mathrm{h}_{N_2}) \\ = 1(-124733 + 0) + 5.2(0 + 0) + 5.2 * 3.76(0 + 0) \end{aligned}$$

$$1.4\Delta \mathrm{h}_{CO_2} + 5\Delta \mathrm{h}_{H_2O} + 2.6\Delta \mathrm{h}_{co} + 19.552\Delta \mathrm{h}_{N_2} = 1{,}922{,}863$$

By trial and error find Tad , try T=2300 K

$$1.4(109670)_{CO_2} + 5(88426)_{H_2O} + 2.6(67682)_{co} + 19.552(66997)_{N_2} = 2{,}081{,}566$$

This is too high, so try T=2100 K

$$1.4(97477)_{CO_2} + 5(77952)_{H_2O} + 2.6(60371)_{co} + 19.552(59738)_{N_2} = 1{,}851{,}189$$

This is too low , so ***Tad*** is found by interpolation

Tad* 2162 *K

Ex4: Estimate the constant – pressure adiabatic flame temperature for combustion of a stoichiometric **CH_4** air mixture .P=1atm and **T** initial 298 K. use the following assumptions

1-complete combustion (no dissociation) (CO2 , H2O ,N2).

2- the ***Cp*** of product estimated at 1200 K (T1+Tad)/2 where Tad about 2100K.

Sol:

$$CH_4 + 2(O_2 + 3.76N_2) \longrightarrow CO_2 + 2H_2O + 2 * 3.76N_2$$

Species	Enthalpy of Formation @ 298 K $h^o_{f,i}$ (kJ/kmol)	Specific Heat @ 1200 K $\bar{c}_{p,i}$ (kJ/kmol-K)
CH_4	−74,831	---
CO_2	−393,546	56.21
H_2O	−241,845	43.87
N_2	0	33.71
O_2	0	---

$$Q = H_{prod} - H_{reac} = 0 \quad \therefore \quad H_{prod} = H_{reac}$$

$$H_{reac} = \sum_{Reca} n_i(h_{f^0} + \Delta \text{h})_i = 1(-74{,}831) + 2(0) + 7.52(0)$$

$$= -74{,}831 \text{ kJ/Kmole}$$

$$H_{prod} = \sum_{prod} n_i(h_{f^0} + \Delta \text{h})_i = n_i(h_{f^0} + \text{C}_p(T_{ad} - 298)_i = 1(-393{,}546 + 56.21(T_{ad} - 298) + 2(-241{,}845 + 43.87(T_{ad} - 298) + 7.52(0 + 33.7(T_{ad} - 298) =? ?$$

$$H_{reac} = H_{prod}$$

$$T_{ad} = 2318\,K$$

In the above, we dealt with a constant-pressure system, which would be appropriate in dealing with a gas-turbine combustor, or a furnace. Let us look now at **constant-volume adiabatic flame temperatures**, which we might require in an ideal Otto-cycle analysis, for example. The first law of thermodynamics requires

$$U_{\text{reac}}(T_{\text{init}}, P_{\text{init}}) = U_{\text{prod}}(T_{ad}, P_f), \qquad 1$$

where U is the absolute (or standardized) internal energy of the mixture. Graphically, Eqn. 1 resembles the sketch 1 used to illustrate the constant-pressure adiabatic flame temperature, except the internal energy replaces the enthalpy. Since most compilations or calculations of thermodynamic properties provide values for H (or h) rather than U (or u) [1, 6], we can rearrange Eqn. 1 to the following form:

$$H_{\text{reac}} - H_{\text{prod}} - V(P_{\text{init}} - P_f) = 0. \qquad 2$$

We can apply the ideal-gas law to eliminate the PV terms:

$$P_{\text{init}} V = \sum_{\text{reac}} N_i R_u T_{\text{init}} = N_{\text{reac}} R_u T_{\text{init}}$$

$$P_f V = \sum_{\text{prod}} N_i R_u T_{ad} = N_{\text{prod}} R_u T_{ad}.$$

Thus,

$$H_{\text{reac}} - H_{\text{prod}} - R_u(N_{\text{reac}} T_{\text{init}} - N_{\text{prod}} T_{ad}) = 0. \qquad 3$$

An alternative form of Eqn. 3, on a per-mass-of-mixture basis, can be obtained by dividing Eqn. 3 by the mass of mixture, m_{mix}, and recognizing that

$$m_{\text{mix}}/N_{\text{reac}} \equiv MW_{\text{reac}}$$

or

$$m_{\text{mix}}/N_{\text{prod}} \equiv MW_{\text{prod}}.$$

We thus obtain

$$h_{\text{reac}} - h_{\text{prod}} - R_u\left(\frac{T_{\text{init}}}{MW_{\text{reac}}} - \frac{T_{ad}}{MW_{\text{prod}}}\right) = 0. \qquad 4$$

Ex5: Estimate the constant – volume adiabatic flame temperature for combustion of a stoichiometric **CH_4** air mixture .P=1atm and **T** initial 298 K. use the same assumptions as in Ex4.

Sol:

$$H_{reac} - H_{prod} - R_u\left(N_{reac} * T_{init} - N_{prod} * T_{ad}\right) = 0$$

$$\sum_{reac} n_i(h)_i - \sum_{prod} n_i(h)_i - R_u\left(N_{reac} * T_{init} - N_{prod} * T_{ad}\right) = 0$$

$$H_{reac} = \sum_{Reca} n_i(h_{f^0} + \Delta\mathrm{h})_i = 1(-74{,}831) + 2(0) + 7.52(0)$$
$$= -74{,}831\ \mathrm{kJ/Kmole}$$

$$\sum_{prod} n_i(h_{f^0} + \Delta\mathrm{h})_i = n_i(h_{f^0} + \mathrm{C}_p(T_{ad} - 298)_i$$

$$H_{prod} = \sum_{prod} n_i(h_{f^0} + \Delta\mathrm{h})_i = n_i(h_{f^0} + \mathrm{C}_p(T_{ad} - 298)_i$$
$$= 1(-393{,}546 + 56.21(T_{ad} - 298)$$
$$+ 2(-241{,}845 + 43.87(T_{ad} - 298)$$
$$+ 7.52(0 + 33.7(T_{ad} - 298)$$
$$= -887{,}236 + 397.5(T_{ad} - 298)$$

$$R_u\left(N_{reac} * T_{init} - N_{prod} * T_{ad}\right) = 8{,}315(10.52)(T_{ad} - 298)$$

$$-74{,}831 - 887{,}236 + 397.5(T_{ad} - 298) - 8{,}315(10.52)(T_{ad} - 298) = 0$$

$$T_{ad} = 2889\ K$$

(i) For the same initial conditions, constant-volume combustion results in much higher temperatures (571 K higher in this example) than for constant-pressure combustion. This is a consequence of the pressure forces doing no work when the volume is fixed. (ii) Note, also, that the number of moles was conserved in going from the initial to final state. This is a fortuitous result for CH_4 and does not occur for other fuels. (iii) The final pressure is well above the initial pressure: $P_f = P_{\mathrm{init}}(T_{ad}/T_{\mathrm{init}}) = 9.69\ \mathrm{atm}$.

H.W: Determine adiabatic flame temperature for constant pressure combustion for **propane** burned with 20% excess of air can assumed that the reactants at 298 k

Lecture No (5)

Classifications of engines and their performance

1. Class: third Year

2. Subject: Classifications of engines and their performance
3. Number of weeks: Two week

4. Central idea: Classifications of engines and their performance
5. The Test:

ENGINE CLASSIFICATIONS

Internal combustion engines can be classified in a number of different ways:

1. Types of Ignition

(a) Spark Ignition (SI). An SI engine starts the combustion process in each cycle by use of a spark plug. The spark plug gives a high-voltage electrical discharge between two electrodes which ignites the air-fuel mixture in the combustion chamber surrounding the plug. **In** early engine development, before the invention of the electric spark plug, many forms of torch holes were used to initiate combustion from an external flame.

(b) Compression Ignition (CI). The combustion process in a CI engine starts when the air-fuel mixture self-ignites due to high temperature in the combustion chamber caused by high compression.

2. Engine Cycle

(a) Four-Stroke Cycle. A four-stroke cycle experiences four piston movements over two engine revolutions for each cycle.

(b) Two-Stroke Cycle. A two-stroke cycle has two piston movements over one revolution for each cycle.

3. Basic Design

(a) Reciprocating. Engine has one or more cylinders in which pistons reciprocate back and forth. The combustion chamber is located in the closed end of each cylinder. Power is delivered to a rotating output crankshaft by mechanical linkage with the pistons

(b) Rotary. Engine is made of a block (stator) built around a large non-concentric rotor and crankshaft. The combustion chambers are built into the nonrotating block.

4. Position and Number of Cylinders of Reciprocating Engines (Fig. 1)

(a) Single Cylinder. Engine has one cylinder and piston connected to the crankshaft.

(b) In-Line. Cylinders are positioned in a straight line, one behind the other along the length of the crankshaft. They can consist of 2 to 11 cylinders or possibly more. In-line four-cylinder engines are very common for automobile and other applications. In-line six and eight cylinders are historically common automobile engines. In-line engines are sometimes called **straight** (e.g., straight six or straight eight).

(c) V Engine. Two banks of cylinders at an angle with each other along a single crankshaft. The angle between the banks of cylinders can be anywhere from 15° to 120°, with 60°-90° being common. V engines have even numbers of cylinders from 2 to 20 or more. V6s and V8s are common automobile engines, with V12s and V16s (historic) found in some luxury and high-performance vehicles.

(d) Opposed Cylinder Engine. Two banks of cylinders opposite each other on a single crankshaft (a V engine with a 180°V). These are common on small aircraft and some automobiles with an even number of cylinders from two to eight or more. These engines are often called flat engines (e.g., flat four).

(e) **W Engine**. Same as a V engine except with three banks of cylinders on the same crankshaft. Not common, but some have been developed for racing automobiles, both modern and historic. Usually 12 cylinders with about a *60°* angle between each bank.

(L) Opposed Piston Engine. Two pistons in each cylinder with the combustion chamber in the center between the pistons. A single-combustion process causes two power strokes at the same time, with each piston being pushed away from the center and delivering power to a separate crankshaft at each end of the cylinder. Engine output is either on two rotating crankshafts or on one crankshaft incorporating complex mechanical linkage.

(g) Radial Engine. Engine with pistons positioned in a circular plane around the central crankshaft. The connecting rods of the pistons are connected to a master rod which, in turn, is connected to the crankshaft. A bank of cylinders on a radial engine always has an odd number of cylinders ranging from 3 to 13 or more. Operating on a four-stroke cycle, every other cylinder fires and has a power stroke as the crankshaft rotates, giving a smooth operation. Many medium- and large-size propeller-driven aircraft use radial engines. For large aircraft, two or more banks of cylinders are mounted together, one behind the other on a single crankshaft, making one powerful, smooth engine. Very large ship engines exist with up to 54 cylinders, six banks of 9 cylinders each.

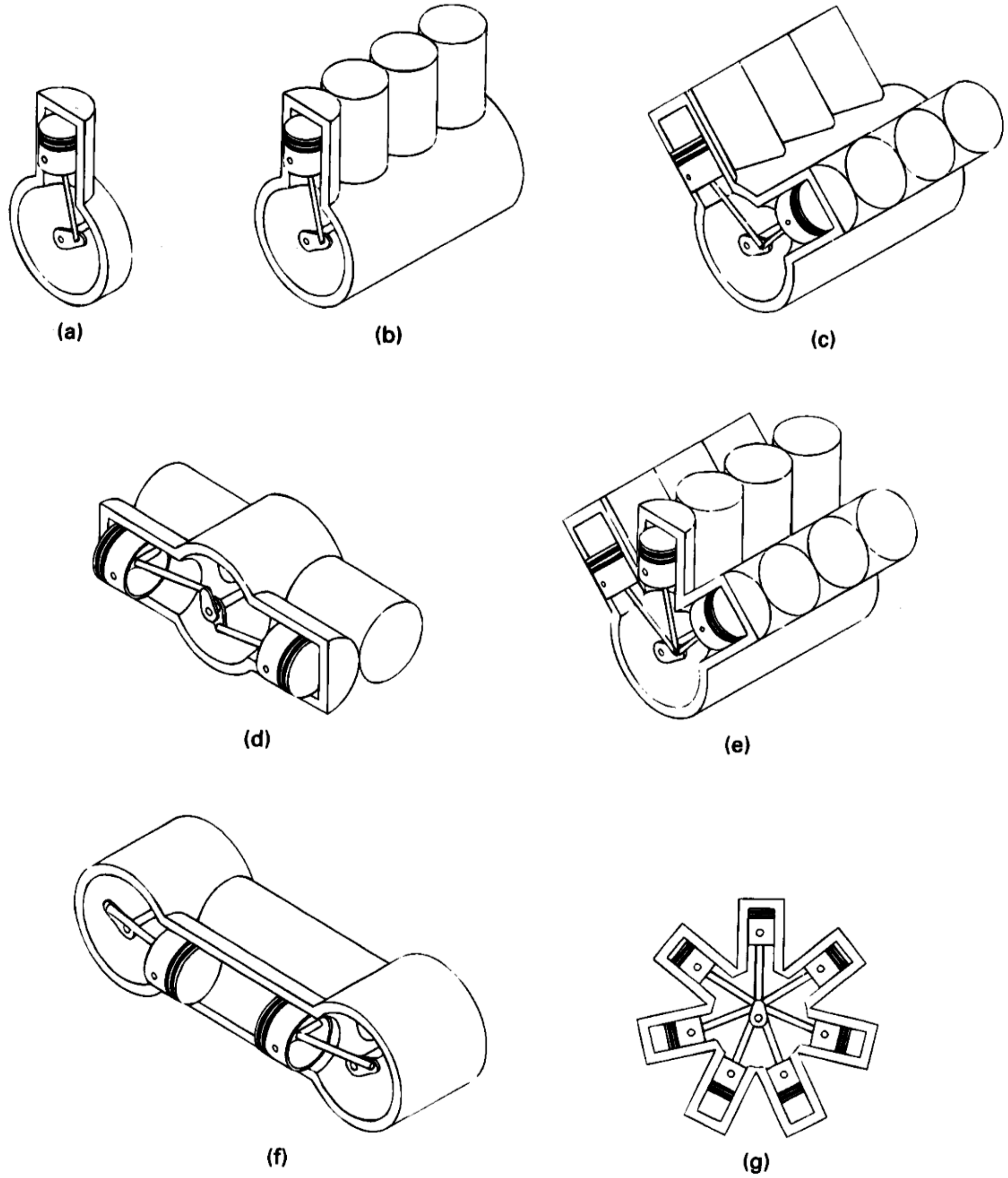


Figure 1 Engine Classification by Cylinder Arrangement. **(a)** Single cylinder. **(b)** In-line, or straight. **(c)** V engine. **(d)** Opposed cylinder. **(e)** W engine. **(f)** Opposed piston. **(g)** Radial.

5. Air Intake Process

(a) Naturally Aspirated. No intake air pressure boost system.

(b) Supercharged. Intake air pressure increased with the compressor driven off of the engine crankshaft

(c) Turbocharged. Intake air pressure increased with the turbine-compressor driven by the engine exhaust gases .

(d) Crankcase Compressed. Two-stroke cycle engine which uses the crankcase as the intake air compressor. Limited development work has also been done on design and construction of four-stroke cycle engines with crankcase compression.

6. Method of Fuel Input for SI Engines

(a) Carbureted.

(b) Multipoint Port Fuel Injection. One or more injectors at each cylinder intake.

(c) Throttle Body Fuel Injection. Injectors upstream in intake manifold.

7. Fuel Used

(a) Gasoline.

(b) Diesel Oil or Fuel Oil.

(c) Gas, Natural Gas, Methane.

(d) LPG.

(e) Alcohol-Ethyl, Methyl.

(f) Dual Fuel. There are a number of engines that use a combination of two or more fuels. Some, usually large, CI engines use a combination of methane and diesel fuel. These are attractive in developing third-world countries because of the high cost of diesel fuel. Combined gasoline-alcohol fuels are becoming more common as an alternative to straight gasoline automobile engine fuel.

(g) Gasohol. Common fuel consisting of 90% gasoline and 10% alcohol.

8. Application

(a) Automobile, Truck, Bus.

(b) Locomotive.

(c) Stationary.

(d) Marine.

(e) Aircraft.

(f) Small Portable, Chain Saw, Model Airplane.

10-Type of Cooling

(a) Air Cooled.

(b) Liquid Cooled, Water Cooled.

Several or all of these classifications can be used at the same time to identify a given engine. Thus, a modern engine might be called a turbocharged, reciprocating, spark ignition, four-stroke cycle, overhead valve, water-cooled, gasoline, multipoint fuel-injected, V8 automobile engine

Engine performance

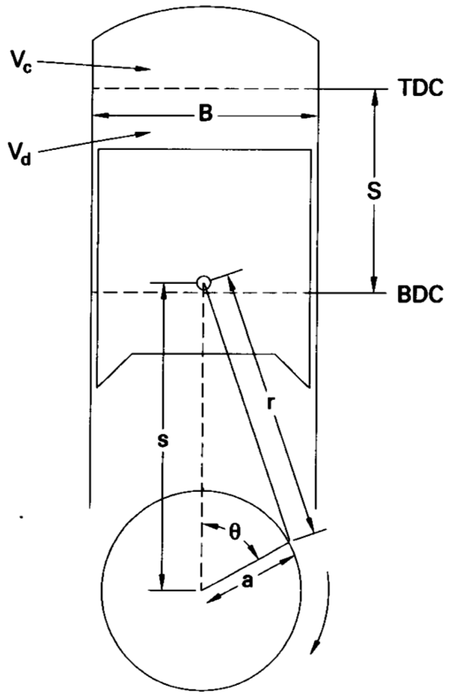
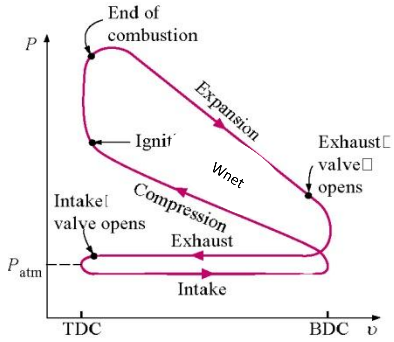


Figure 2 Piston and cylinder geometry of reciprocating engine. B = bore; S = stroke; r = connecting rod length; a = crank offset; s = piston position; θ = crank angle; V_c = clearance volume; V_d = displacement volume.



1) Brake power

$$B_p = \frac{2\pi NT}{60*1000} \quad \text{…………. (1)}$$

Bp: Brake power (KW)

N: speed (r.p.m)

T:Torque (n.m)

$$B_p = \dot{m}_f * L.C.V * \eta_{bth} \quad \text{………… (2)}$$

$\dot{m}_f$: mass flow rate of fuel (kg/s)

L.C.V: lower calorific value (KJ/kg)

η_{bth} : brake thermal efficiency.

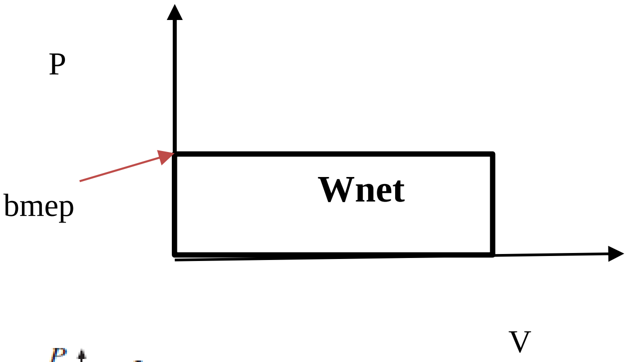
$$\eta_{bth} = \frac{B_p}{\dot{m}_f * L.V.C} \quad \ldots\ldots\ldots\ldots\ (2a)$$

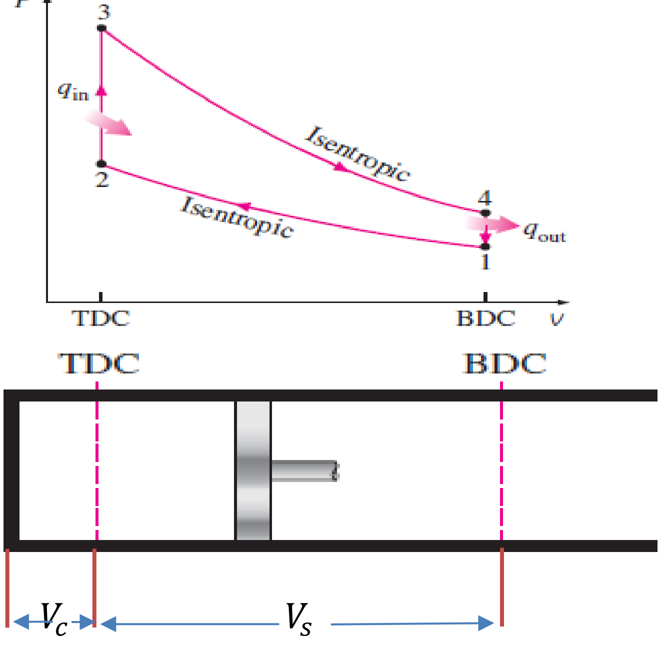
$$B_p = bmep * \dot{V}_s * 10^2 \ \ldots\ldots\ldots(3)$$

$\dot{V}_s$: swept volume (m³/sec)

bemp: brake mean effective pressure (bar): t is hypothetical pressure if it was placed on the piston in the power stroke, it would not give us the same net work that could be obtained a full turn.

$$bmep = \frac{W_{net}}{(V_1 - V_2) * 10^2} \ldots (4)$$





$$V_s = \frac{\dot{\pi} B^2}{4} * L$$

$$\dot{V}_s = \frac{\pi B^2}{4} * \dot{L} * C * \frac{N}{60 * Z}$$

$\dot{V}_s$: swept volume (m³/sec)

V_C: clearance volume (m³/sec)

L: stroke (m)

B:diameter of cylinder (bore)(m)

C:number of cylinder

Z:crank shaft revolution for complete power cycle

Z=2 four stroke cycle

Z=1 two stroke cycle

$$r = \frac{V_s+V_c}{V_c}$$

r: Compression ratio

2- Indicate power Ip (KW)

$$I_p = \dot{m}_f * L.C.V * \eta_{Ith} \text{ .... (5)}$$

$\dot{m}_f$: mass flow rate of fuel (kg/s)

η_{bth} : Indicate thermal efficiency

$$I_p = Imep * \dot{V}_s * 10^2 \text{ ....(6)}$$

brake mean effective pressure (bar)

3) Specific fuel consumption (kg/Kw.hr)

a) Brake specific fuel consumption (b.s.f.c)

$$b.s.f.c = \frac{\dot{m}_f}{B_p} \text{ ....(7)}$$

$$\dot{m}_f = B_p * b.s.f.c \qquad (Kg/hr)$$

$$\dot{m}_f = \frac{B_p * b.s.f.c}{3600} \qquad (Kg/sec)$$

b) Indicated specific fuel consumption (b.s.f.c)

$$I.s.f.c = \frac{\dot{m}_f}{I_p} \ldots\ldots\ldots\ldots(8)$$

4) Mechanical efficiency η_m

$$\eta_m = \frac{B_p}{I_p}$$

$$\eta_m = \frac{\dot{m}_f * L.C.V * \eta_{bth}}{\dot{m}_f * L.C.V * \eta_{Ith}} = \frac{\eta_{bth}}{\eta_{Ith}} = \frac{b.s.f.c}{I.s.f.c} = \frac{bmep}{Imep} \ldots.(9)$$

5) Volumetric efficiency η_V: the ratio of the air induced measured at the free air conditions to the swept volume of the cylinder

$$\eta_V = \frac{(\dot{m}_{air})_{actual}}{(\dot{m}_{air})_{ideal}} \ldots\ldots(10)$$

$$(\dot{m}_{air})_{ideal} = \rho_{air} * \dot{V}_s$$

$$\eta_V = \frac{\dot{m}_{air}}{\rho_{air} * \dot{V}_s}$$

$$\rho_{air} = \frac{P * 10^2}{RT}$$

$\eta_{bth}=(0.25-0.33)$

$\eta_{ith}=(0.26-0.38)$

$\eta_{m}=(0.7-0.95)$

$\eta_{V}=(0.6-0.96)$

Ex1: a 2-stroke diesel engine has a capacity of 1.8 liter . if the (s.f.c) is 0.3 kg/kw.hr and the engine develops a torque of 100 N.m at 2000 r.p.m calculate the volumetric and brake thermal efficiency , given that (A/F) 30/1

L.C.V =4000 KJ/kg and ambient conditions are p=1.013 bar , T=25ºC .

Sol:

$$B_p = \frac{2\pi NT}{60*1000} = \frac{2\pi*2000*100}{60*1000} = 20.9KW$$

$$B_p = \dot{m}_f * L.V.C * \eta_{bth}$$

$$b.s.f.c = \frac{\dot{m}_f}{B_p} = 0.3 = \frac{\dot{m}_f}{20.9} \Longrightarrow \dot{m}_f = 6.28\, Kg/hr$$

$$\dot{m}_f = \frac{6.28}{3600} = 0.00174\, kg/sec$$

$$\eta_{bth} = \frac{B_p}{\dot{m}_f * L.C.V} = \frac{20.9}{0.0017 * 40000} = 0.0 = 299 = 29.9\%$$

$$\eta_V = \frac{(\dot{m}_{air})_{actual}}{(\dot{m}_{air})_{ideal}}$$

$$(\dot{m}_{air})_{ideal} = \rho_{air} * \dot{V}_s$$

$$\dot{V}_s = V_s * \frac{N}{60 * z} = 1.8 * 10^{-3} * \frac{2000}{60 * 1} = 0.26\, m^3/sec$$

$$\rho_{air} = \frac{P * 10^2}{RT} = \frac{1.013 * 10^2}{0.287 * 298} = 1.184\, kg/m^3$$

$$\frac{A}{F} = \frac{\dot{m}_{air}}{\dot{m}_f}$$

$$30 = \frac{\dot{m}_{air}}{0.00174} \Longrightarrow \dot{m}_{air} = 0.0522\, kg/sec$$

$$\eta_V = \frac{\dot{m}_{air}}{\rho_{air} * \dot{V}_s} = \frac{0.0522}{1.184 * 0.06} = 0.73 = 73\%$$

Ex2: a-4 cylinder 4-stroke diesel engine has a bore =21 cm and stroke L= 29cm .and running at 720 r.p.m .the bmep =6 bar , and b.s.f.c is 0.23 kg/kw.hr . the (A/F) is 24/1. calculate the η_{bth} , η_V and η_{Ith} given ambient conditions are P= 1 bar , T=15ºC, L.C.V of fuel is 44000 KJ/Kg and $\eta_m = 80\%$.

Sol:

$$\dot{V}_s = \frac{\pi B^2}{4} * L * C * \frac{N}{60 * Z} = \frac{\pi (0.21)^2}{4} * 0.29 * 4 * \frac{720}{60 * 2} = 0.24\, m^3/s$$

$$B_p = bmep * \dot{V}_s * 10^2 = 6 * 0.24 * 10^2 = 144\, KW$$

$$B_p = \dot{m}_f * L.C.V * \eta_{bth}$$

$$b.s.f.c = \frac{\dot{m}_f}{B_p} = 0.23 = \frac{\dot{m}_f}{144} \Longrightarrow \dot{m}_f = \frac{144 * 0.23}{3600} = 0.0092\, Kg/s$$

$$\eta_{bth} = \frac{144}{0.0092 * 44000} = 0.35 = 35\%$$

$$\eta_m = \frac{\eta_{bth}}{\eta_{ith}} \Longrightarrow \eta_{ith} = \frac{0.35}{0.8} = 0.437 = 43.7\%$$

$$\frac{A}{F} = \frac{\dot{m}_{air}}{\dot{m}_f}$$

$$24 = \frac{\dot{m}_{air}}{0.0092} \Longrightarrow \dot{m}_{air} = 0.2208\,kg/sec$$

$$\rho_{air} = \frac{P * 10^2}{RT} = \frac{1.01 * 10^2}{0.287 * 298} = 1.22\,kg/m^3$$

$$\eta_V = \frac{\dot{m}_{air}}{\rho_{air} * \dot{V}_s} = \frac{0.2208}{1.22 * 0.24} = 0.75 = 75\%$$

Air-Standard Assumptions

In our study of gas power cycles, we assume that the working fluid is air, and the air undergoes a thermodynamic cycle even though the working fluid in the actual power system does not undergo a cycle.

To simplify the analysis, we approximate the cycles with the following assumptions:

- The air continuously circulates in a closed loop and always behaves as an ideal gas.
- All the processes that make up the cycle are internally reversible.
- The combustion process is replaced by a heat-addition process from an external source.
- A heat rejection process that restores the working fluid to its initial state replaces the exhaust process.
- The cold-air-standard assumptions apply when the working fluid is air and has constant specific heat evaluated at room temperature (25^{o}C or 77^{o}F).

Terminology for Reciprocating Devices

- The following is some terminology we need to understand for reciprocating engines—typically piston-cylinder devices. Let’s look at the following figures for the definitions of top dead center (TDC), bottom dead center (BDC), stroke, bore, intake valve, exhaust valve, clearance volume, displacement volume, compression ratio, and mean effective pressure.

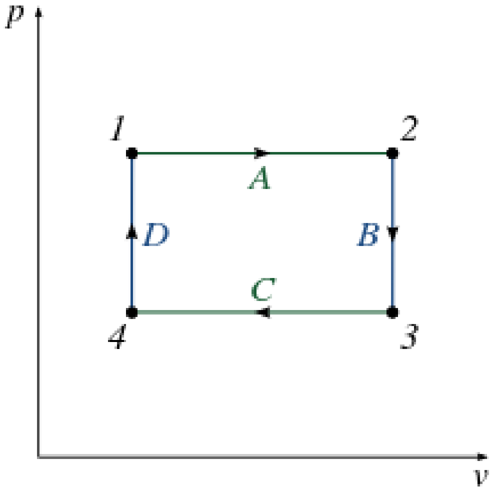
Pressure-Volume Diagrams

A pressure volume diagram (or PV diagram, or volume-pressure loop) is used to describe corresponding changes in volume and pressure in a system. They are commonly used in thermodynamics,

PV diagrams, originally called indicator diagrams, were developed in the 18th century as tools for understanding the efficiency of steam engines.

A PV diagram plots the change in pressure *P* with respect to volume *V* for some process or processes. Typically in thermodynamics, the set of processes forms a cycle, so that upon completion of the cycle there has been no net change in state of the system; i.e. the device returns to the starting pressure and volume.

The figure shows the features of a typical PV diagram. A series of numbered states (1 through 4) are noted. The path between each state consists of some process (A through D) which alters the pressure or volume of the system (or both).



A key feature of the diagram is that the amount of energy expended or received by the system as work can be estimated as the area under the curve on the chart. For a cyclic diagram, the net work is that *enclosed* by the curve. In the example given in the figure, the processes 1-2-3 produce a work output, but processes from 3-4-1 require a smaller energy input to return to the starting position / state; thus the net work is the difference between the two.

Note that this figure is highly idealized, and a diagram showing the processes in a real device would tend to depict a more complex shape of the PV curve.

Mean process on p-v diagram

Recall from the previous section…

$$\Delta U = Q + W$$

$Q > 0$	system absorbs heat from the environment
$Q < 0$	system releases heat to the environment
$W > 0$	work done on the system by the environment
$W < 0$	work done by the system on the environment

A system can be described by three thermodynamic variables. — pressure, volume, and temperature. Well, maybe it's only two variables. With everything tied together by the ideal gas law, one variable can always be described as dependent on the other two.

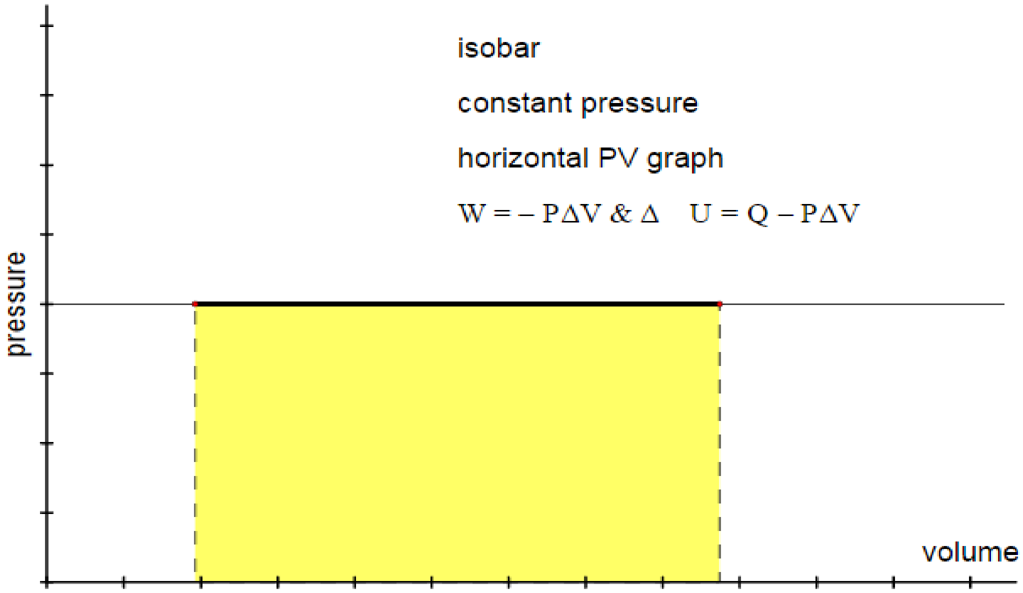
$$PV=mRT$$

Curves

isobaric

- constant pressure
- "bar" comes from the Greek word for heavy: βαρύς [*varys*]
- examples: weighted piston, flexible container in earth's atmosphere, hot air balloon
- PV graph is a horizontal line

$W = -P\Delta V \Rightarrow \Delta U = Q - P\Delta V$



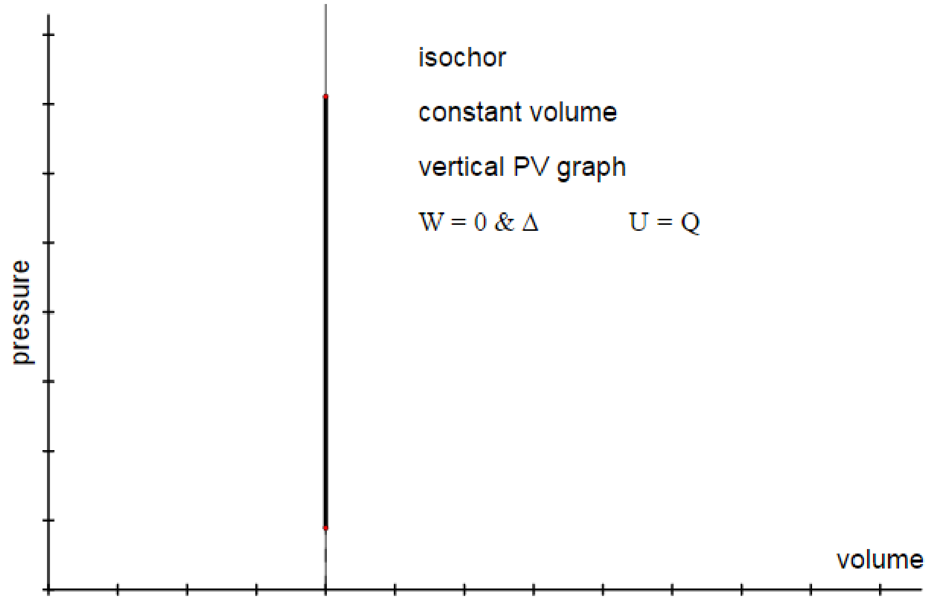
$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \quad , \quad Q = mc_p(T_2 - T_1) \quad , \frac{p_1V_1}{T_1} = \frac{p_2V_2}{T_2}$$

PV=mRT

isochoric

- constant volume
- "chor" comes from the Greek word for volume: χώρος [*khoros*]
- examples: closed rigid container, constant volume thermometer
- PV graph is a vertical line

$$W = 0 \Rightarrow \Delta U = Q$$



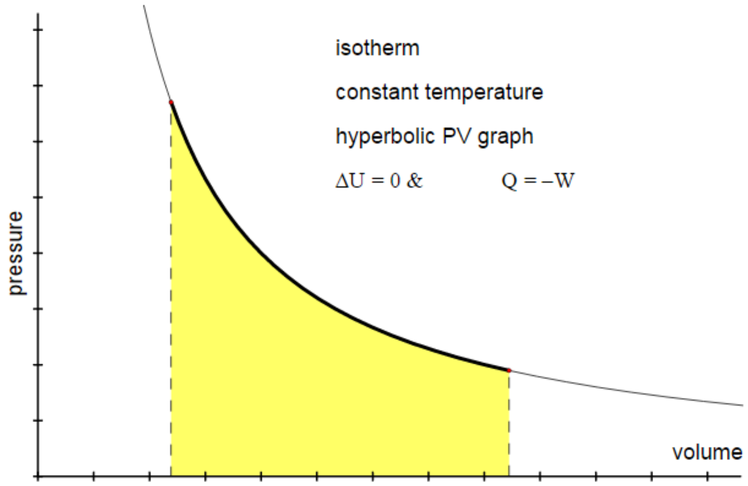
$$Q = mc_v(T_2 - T_1) \quad , \frac{p_1V_1}{T_1} = \frac{p_2V_2}{T_2}$$

PV=mRT

isothermal

- constant temperature
- "therm" comes from the greek work for heat: θερμότητα [*thermotita*]
- examples: "slow" processes, breathing out through a wide open mouth
- PV graph is a rectangular hyperbola

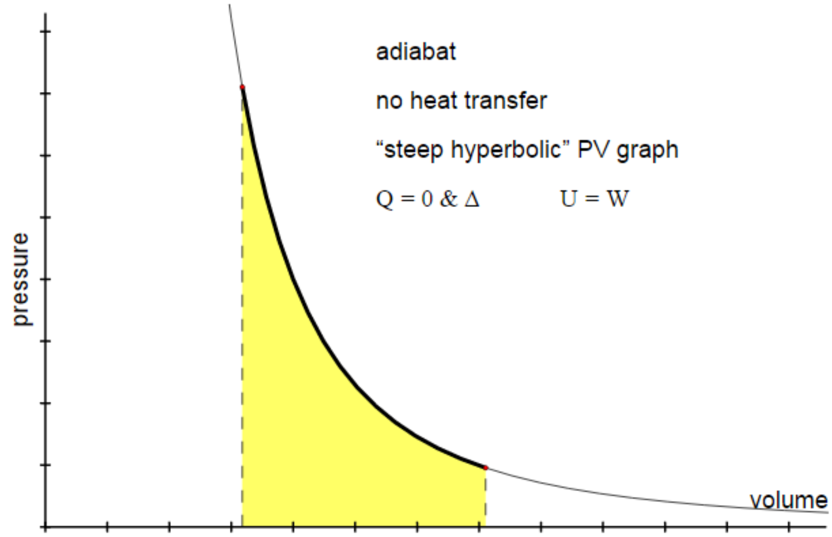
$\Delta U = 0 \Rightarrow Q = -W$



adiabatic

- no heat exchange with the environment
- adiabatic has a complex Greek origin that means "not + through +go": α + Δια + βατός [*a* + *dia* + *vatos*]
- examples: "fast" processes, forcing air out through pursed lips, bicycle tire pump
- PV diagram is a "steep hyperbola"

$Q = 0 \Rightarrow \Delta U = W$



$$P_1V_1^{\gamma} = P_2V_2^{\gamma} \quad , \quad \frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} \quad , \quad \frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}}$$

whereas(γ) gas index is $\gamma = \frac{C_p}{C_V}$

For air γ=1.4 , $C_p = 1.005\, kJ/Kg.k$, $C_V = 0.717\, kJ/Kg.k$

R=287 J/Kg. K

Lecture No (7)

Otto Cycle

1. Class: third Year

2. Subject: Otto Cycle

3. Number of weeks: one week

4. Central idea: Otto Cycle

5. The Test:

Otto Cycle: The Ideal air standard Cycle for Spark-Ignition Engines (petrol engine)

Consider the automotive spark-ignition power cycle.

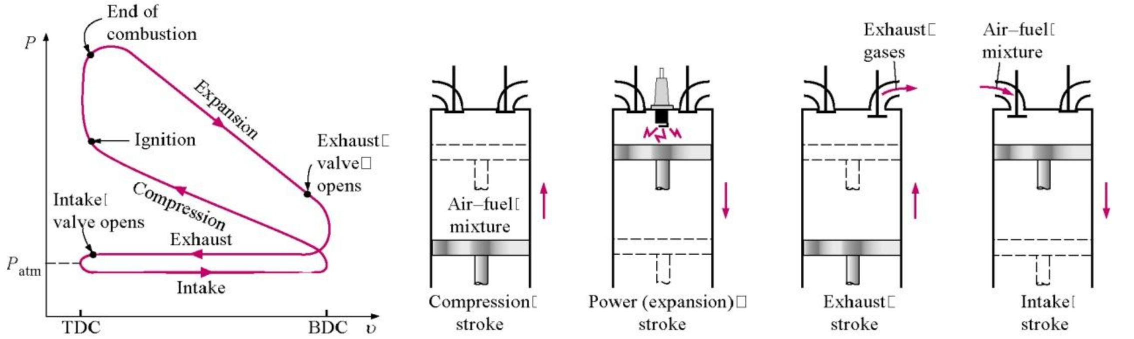
Processes

Intake stroke

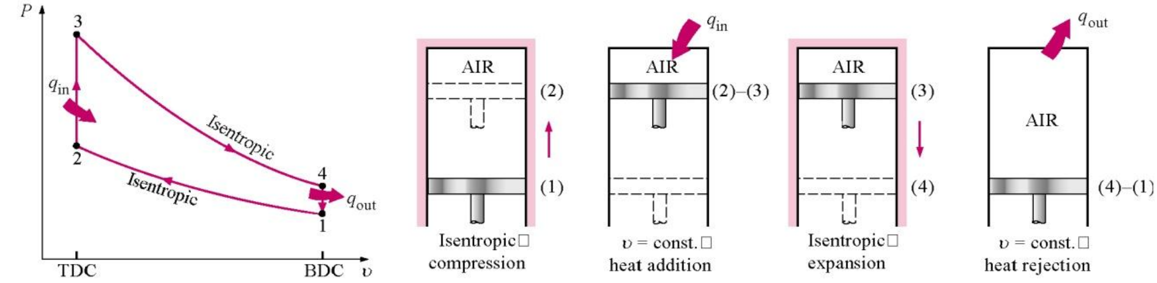
Compression stroke

Power (expansion) stroke

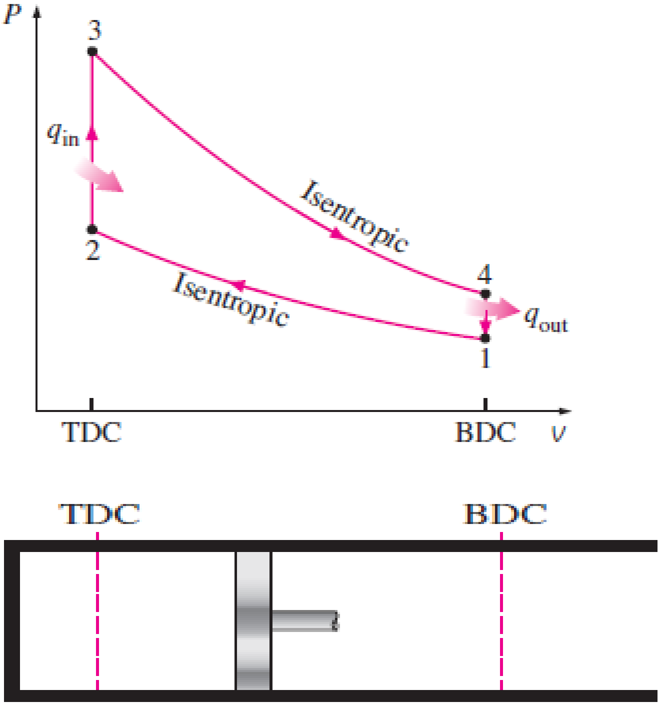
Exhaust stroke



(a) Actual four-stroke spark-ignition engine



(b) Ideal Otto cycle



Process 1-2 isentropic compression (piston moves from BDC to TDC gas compressed isentropically pv^{γ}=c.

Process 2-3 constant volume heat adding (at the TDC ,the piston is kept at rest instantaneous , combustion occurs , heat adding at constant volume .

Process 3-4 isentropic expansion (the piston returns to the BDC, gas is expanded isentropically pv^{γ}=c.

Process 4-1 constant volume heat rejection (piston kept at rest heat is rejected from gas at constant volume until the initial condition is attained .

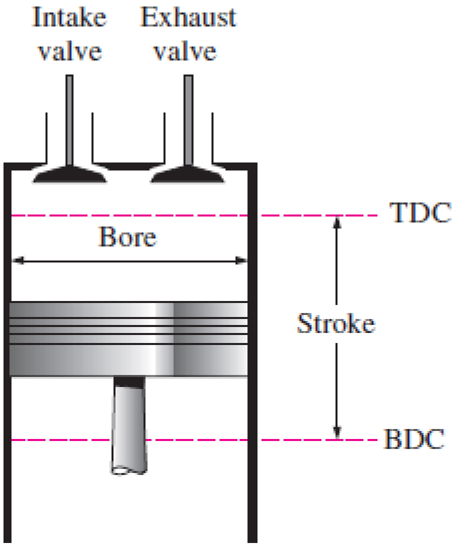
Compression ratio :the ratio of the maximum volume formed in the cylinder to the minimum (clearance) volume

$$r = \frac{Vmax}{Vmin} = \frac{V1}{V2}$$

$$r = \frac{swept\ volume + clearance\ volume}{clearance\ volume}$$

$$r = \frac{V_s + V_c}{V_c}$$

$$V_s = \frac{\pi}{4} D^2 L$$



TDC: Top died center

BDC: Bottom died center

V_s: *swept volume*

V_c: *clearance volume*

L:stroke

D: diameter of cylinder (bore)

Thermal efficiency of the ideal Otto cycle :

$$\eta_{otto} = \frac{w_{net}}{Q_{add}} = \frac{Q_{add} - Q_{rej}}{Q_{add}}$$

$$\eta_{otto} = 1 - \frac{Q_{rej}}{Q_{add}}$$

$$Q_{add} = mc_v(T_3 - T_2)$$

$$Q_{rej} = mc_v(T_4 - T_1)$$

$$\eta_{Otto} = 1 - \frac{mc_v(T_4 - T_1)}{mc_v(T_3 - T_2)} = 1 - \frac{(T_4 - T_1)}{(T_3 - T_2)}$$

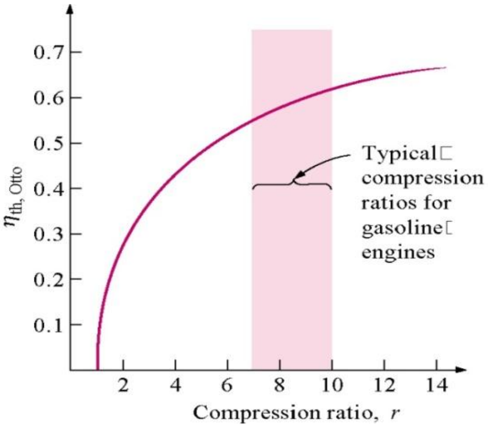
$$\eta_{Otto} = 1 - \frac{mc_v(T_4 - T_1)}{mc_v(T_3 - T_2)} = 1 - \frac{T_1\left(\frac{T_4}{T_1} - 1\right)}{T_2\left(\frac{T_3}{T_2} - 1\right)}$$

Process (1-2)

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = r^{\gamma-1}$$

Process (3-4)

$$\frac{T_3}{T_4} = \left(\frac{V_4}{V_3}\right)^{\gamma-1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = r^{\gamma-1}$$



$$V_4 = V_1$$

$$V_3 = V_2 \qquad \therefore \frac{T_2}{T_1} = \frac{T_3}{T_4} \Longrightarrow \frac{T_4}{T_1} = \frac{T_3}{T_2}$$

$$\eta_{otto} = 1 - \frac{T_1}{T_2} \qquad \frac{T_1}{T_2} = \left(\frac{V_2}{V_1}\right)^{\gamma-1} = \frac{1}{r^{\gamma-1}}$$

$$\eta_{otto} = 1 - \frac{1}{r^{\gamma-1}}$$

We see that increasing the compression ratio increases the thermal efficiency. However, there is a limit on *r* depending upon the fuel. Fuels under high temperature resulting from high compression ratios will prematurely ignite, causing knock.

Example(1):Calculate the thermal efficiency of Otto cycle with a cylinder bore of (50 mm) and stroke of (75 mm) .and a clearance volume of 21.3 cm^3

Sol :

$$\eta_{otto} = 1 - \frac{1}{r^{\gamma-1}}$$

$$r = \frac{Vmax}{Vmin} = \frac{V1}{V2}$$

$$r = \frac{swept\ volume + clearance\ volume}{clearance\ volume}$$

$$V_1 = V_s + V_c$$

$$V_s = \frac{\pi}{4}\ D^2L$$

$$V_s = \frac{\pi}{4}\ (50^2) * 75 = 147.2\ cm^3$$

$$V_1 = 147.2 + 21.3 = 168.2$$

$$r = \frac{168.2}{21.3} = 7.92$$

$$\eta_{otto} = 1 - \frac{1}{7.92^{\gamma-1}} = 56.3\%$$

Example2:) The compression ratio of an air standard Otto cycle is 9 .the pressure and temperature at the beginning of the compression process is 100 Kpa , 30 ºC respectively .and the temperature and volume at the end of expansion process is 800k ,600 cm³ respectively. Determine

1)Maximum pressure and temperature in the cycle.

2)The amount of heat added to the cycle.

3)The thermal efficiency of the cycle.

Sol:

Process 1-2

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = T_2 = 303(9)^{1.4-1} = 729.69\text{k}$$

$$V_1 = V_4 = 0.0006\, m^3$$

$$r = \frac{V_1}{V_2} = \frac{0.0006}{V_2} = 9 \Rightarrow V_2 = 0.0000666 m^3$$

$$P_1 V_1^{\gamma} = P_2 V_2^{\gamma} = 100 * 0.0006^{1.4} = P_2 * 0.0000666^{1.4}$$

$$P_2 = 2170.44\, Kpa$$

Process 3-4

$$\frac{T_3}{T_4} = \left(\frac{V_4}{V_3}\right)^{\gamma-1} = T_3 = 800(9)^{1.4-1} = 1926.57\text{k}$$

Process 2-3

$$\frac{p_3 V_3}{T_3} = \frac{p_2 V_2}{T_2} = p_3 \frac{T_3}{T_2} p_2 = \left(\frac{1926.57}{729.69}\right)(2170.44) = 5730.55\text{Kpa}$$

2-

$$Q_{add} = c_V(T_3 - T_2) = 0.717(1926.57 - 729.69)$$
$$= 858.1629\ KJ/Kg$$

3- $\eta=1-\frac{1}{r^{\gamma-1}} = 1 - \frac{1}{9^{\gamma-1}} = 58.47\%$

Lecture No (8)

diesel cycle

1. Class: third Year

2. Subject: diesel cycle

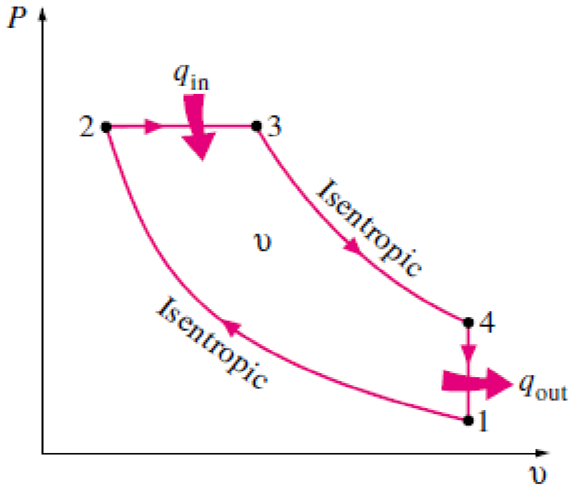
3. Number of weeks: one week

4. Central idea: diesel cycle

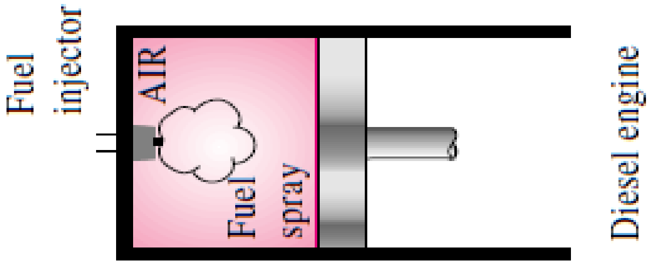
5. The Test:

diesel cycle

The ideal approximation of the diesel compression ignition internal combustion engine is the air standard diesel cycle :



(a) P-υ diagram



Process 1-2 isentropic compression (piston moves from BDC to TDC gas compressed isentropically pv^{γ}=c.

Process 2-3 constant pressure heat adding (at the TDC ,the piston is kept at rest instantaneous , combustion occurs , heat adding at constant pressure .

Process 3-4 isentropic expansion (the piston returns to the BDC, gas is expanded isentropically pv^{γ}=c.

Process 4-1 constant volume heat rejection (piston kept at rest heat is rejected from gas at constant volume until the initial condition is attained .

Volume at Point (3) called cut off volume

Definition :

1-Compression ratio :the ratio of the maximum volume formed in the cylinder to the minimum (clearance) volume .

$$r = \frac{Vmax}{Vmin} = \frac{V1}{V2}$$

2- Expansion ratio (r_e) :the ratio between the volumes in the expansion process (3-4)

$$r_e = \frac{Vmax}{Vcut\ off\ vol} = \frac{V4}{V3}$$

3-Cut off ratio (e) :the ratio of the cylinder volumes after and before the combustion process :

$$e = \frac{Vcutoff\ vol}{Vmin} = \frac{V3}{V2}$$

Put $\frac{r}{e} = \frac{V_1}{V_2} \cdot \frac{V_2}{V_3} = \frac{V_1}{V_3} = \frac{V_4}{V_3} = r_e$

Thermal efficiency of the ideal diesel cycle :

$$\eta_{Diesel} = \frac{w_{net}}{Q_{add}} = \frac{Q_{add} - Q_{rej}}{Q_{add}}$$

$$\eta_{Diesel} = 1 - \frac{Q_{rej}}{Q_{add}}$$

$$Q_{add} = mc_p(T_3 - T_2)$$

$$Q_{rej} = mc_v(T_4 - T_1)$$

$$\eta_{Diesel} = 1 - \frac{mc_v(T_4 - T_1)}{mc_p(T_3 - T_2)} = 1 - \frac{(T_4 - T_1)}{\gamma(T_3 - T_2)}$$

Process (1-2)

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = T_2 = T_1 r^{\gamma-1}$$

$$\frac{T_3}{T_2} = \frac{V_3}{V_2} = e \Rightarrow T_3 = T_2 . e$$

$$T_3 = T_1 r^{\gamma-1} . e$$

Process (3-4)

$$\frac{T_4}{T_3} = \left(\frac{V_3}{V_4}\right)^{\gamma-1} = \left(\frac{1}{r_e}\right)^{\gamma-1} = \left(\frac{e}{r}\right)^{\gamma-1}$$

$$T_4 = T_3\left(\frac{e}{r}\right)^{\gamma-1}$$

$$T_4 = T_1 r^{\gamma-1}\,.\,e.\frac{e^{\gamma-1}}{r^{\gamma-1}}$$

$$T_4 = T_1 e^{\gamma}$$

$$\eta_{Diesel} = 1 - \frac{T_1 e^{\gamma} - T_1}{\gamma[T_1 r^{\gamma-1}.e - T_1 r^{\gamma-1}\,]} \qquad \eta_{Diesel} = 1 - \frac{e^{\gamma}-1}{\gamma r^{\gamma-1}(e-1)}$$

Ex1:-The compression ratio of an air standard diesel cycle is 18 and cutoff ratio 1.5 .at the beginning of the compression stroke the temperature 290 k . determine :-

1-the maximum temperature of the air

2- the heat addition

3-thermal efficiency

Sol:

1- $\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = T_2 = 290(18)^{1.4-1}$=921.5k

$\frac{T_3}{T_2} = \left(\frac{V_3}{V_2}\right) = T_3 = T_2.e = (921.5\ ).(1.5) = 1382\ k$

2-$Q_{add} = c_p(T_3 - T_2) = 1.005(1382 - 921.5) = 462.80\ KJ/Kg$

3- $\eta_{Diesel} = 1 - \frac{e^{\gamma}-1}{\gamma r^{\gamma-1}(e-1)}$

$$\eta_{Diesel} = 1 - \frac{1.5^{1.4} - 1}{1.4\ 18^{1.4-1}(1.5-1)} = 0.6565$$

Ex2: Calculate the thermal efficiency of air standard diesel cycle with a compression ratio of (15) and the maximum and minimum cycle temperature of (1650 ºC) and (15 ºC) respectively .the maximum pressure is (45) bar .the properties of air at room temperature.(cp=1.005Kj/kg.k).(cv=0.718KJ/kg.k).(*R*=0.287 kJ/kg.k) (γ=1.4)

Sol :

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{\gamma-1} = T_2 = 288(15)^{1.4-1} = 850.802\text{k}$$

$$p_3 V_3 = R T_3 \ = 4500 * V_3 = 0.287 * 1923$$

$$V_3 = 0.12264 \frac{m^3}{kg}$$

$$\frac{T_3}{T_2} = \frac{V_3}{V_2} = \frac{1923}{850.802} = \frac{0.12264}{V_2} \quad \Rightarrow V_2 = 0.05426 \frac{m^3}{kg}$$

$$e = \frac{V_3}{V_2} = \frac{0.12264}{0.05426} = 2.262$$

$$\eta_{Diesel} = 1 - \frac{2.262^{1.4} - 1}{1.415^{1.4-1}(2.262-1)} = 0.59 = 59\%$$

Lecture No (9)

Air-fuel cycle

1. Class: third Year

2. Subject: Air-fuel cycle

3. Number of weeks: Two week

4. Central idea: Air-fuel cycle

5. The Test:

Air-fuel cycle

The theoretical cycle based on the actual properties of the cylinder gases is called the (Air-fuel). this cycle may be taken the following consideration.

1- The actual composition of cylinder gases
2- The variation in the specific heat of gases with temperature.(i.e cp & cv not constant)
3- The fact the fuel – air not completely combine chemically at high temperature.
4- The variation in the number molecular present in the cylinder at high temperature.

Air-fuel cycle assumption

1- Fuel is completely vaporized and perfectly mixed with air .
2- Burning or combustion take place at top dead center .
3- Assume no heat exchange occurs between the gases and cylinder wall.
4- Compression and expansion are reversible and charge (air+fuel) transfer happen but work transfer may be ignored .

Definitions :

1- Fresh air (mass flow rate of air) ($\dot{m}_{air}$) : which is the new mass of air supplied to cylinder for each cycle :

$$\dot{m}_{air} = (1 - f) \dots\dots\dots\dots (1)$$

***f*:** Residual gases fraction

2- Fresh fuel ($\dot{m}_{fuel}$) : may be defined as new mass of fuel supplied to the cylinder for each cycle .

$$\boldsymbol{\dot{m}_{fuel} = (1 - f)F \dots\dots\dots\dots (2)}$$

Where :

F= Fuel – Air ratio

$$\boldsymbol{F = \frac{\dot{m}_f}{\dot{m}_{air}} = \frac{1}{\left(\frac{A}{F}\right)}}$$

3- Total charge $\boldsymbol{\dot{m}_T}$:

is the total constant of cylinder at any time of the cycle .

$$\boldsymbol{\dot{m}_T = \dot{m}_{air} + \dot{m}_f + \dot{m}_R}$$

Where

$\boldsymbol{\dot{m}_R}$ **:** Residual mass

$$\boldsymbol{f = \frac{\dot{m}_R}{\dot{m}_m}}$$

4- Fresh mixture ($\dot{\boldsymbol{m}}_{\boldsymbol{i}}$) :

This may be classified according to the type of engine (S.I or C.I)

For **S.I** ($\dot{\boldsymbol{m}}_{\boldsymbol{fresh}} = \dot{\boldsymbol{m}}_{\boldsymbol{air}} + \dot{\boldsymbol{m}}_{\boldsymbol{f}}$)

For **C.I** ($\dot{\boldsymbol{m}}_{\boldsymbol{fresh}} = \dot{\boldsymbol{m}}_{\boldsymbol{air}}$)

Finally : we may summarized then as follows :

$\dot{\boldsymbol{m}}_{\boldsymbol{air}} = (1-f)$

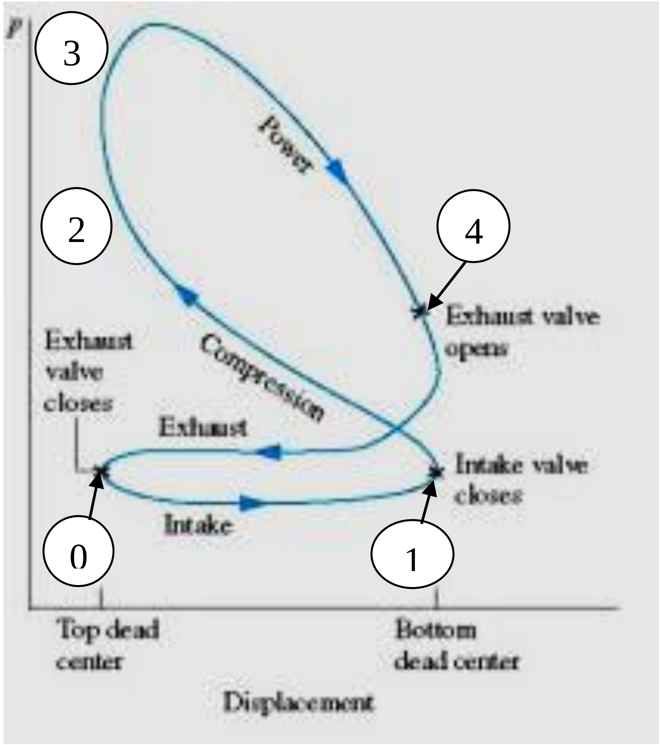
$\dot{\boldsymbol{m}}_{\boldsymbol{f}} = (1-f)F$

$\dot{\boldsymbol{m}}_{\boldsymbol{R}} = (1+F)f$

$\dot{\boldsymbol{m}}_{\boldsymbol{m}} = (1+F)$

The fuel -air cycle

1-constant volume cycle (gasoline engine cycle):



point (4) exhaust valve is opened

$T_4 = T_O = T_{exh}$

point (0) exhaust valve is closed

$P_O = P_1 = P_{exh}$

في حاله دوره محرك البنزين اثناء شوط السحب سوف يدخل(وقود وهواء) مع وجود غازات عادمه داخل الاسطوانه

***f*:** Residual gases fraction

at point (4) $\boldsymbol{T_4 = T_{exh}}$ $\boldsymbol{V_2 = V_O = V_3}$

$$P_4 V_1 = m_m R T_{exh} \;\ldots\ldots\ldots\ldots(1)$$

At point (o)

$$P_{exh} V_2 = m_R R T_{exh}$$

$$P_4 V_1 = (1+F) R T_4 \;\ldots\ldots\ldots\ldots(2)$$

$$P_{exh} V_2 = (1+F) f R T_4 \;\ldots\ldots\ldots(3)$$

نقسم المعادله (2) على (3)

$$\frac{P_4 V_1 = (1+F) R T_4}{P_{exh} V_2 = (1+F) f R T_4}$$

$$\boldsymbol{f = \frac{P_{exh}}{P_4} * \frac{1}{r}}$$

$$r = \frac{V_1}{V_2}$$

$$\boldsymbol{\dot{m}_{air}} = (1-f)$$
$$\boldsymbol{\dot{m}_{f}} = (1-f)F$$
$$\boldsymbol{\dot{m}_{R}} = (1+F)f$$
$$\boldsymbol{\dot{m}_{m}} = (1+F)$$

$$T_2 = T_1 (r)^{\gamma-1} \qquad \gamma_m = \frac{C_{pm}}{C_{V}m}$$

$$C_{pm} = \sum \frac{m_i}{m_m} C_{pi} = \frac{1}{m_m}\left(m_{air} C_{pair} + m_f C_{pf} + m_R C_{pR}\right)$$

$$C_{Vm} = \sum \frac{m_i}{m} C_{Vi}$$

$$R_m = \sum \frac{m_i}{m} R_i$$

$$Q_{add} = m_m c_{cv}(T_3 - T_2)$$

$$Q_{add} = \dot{m}_f * L.C.V$$

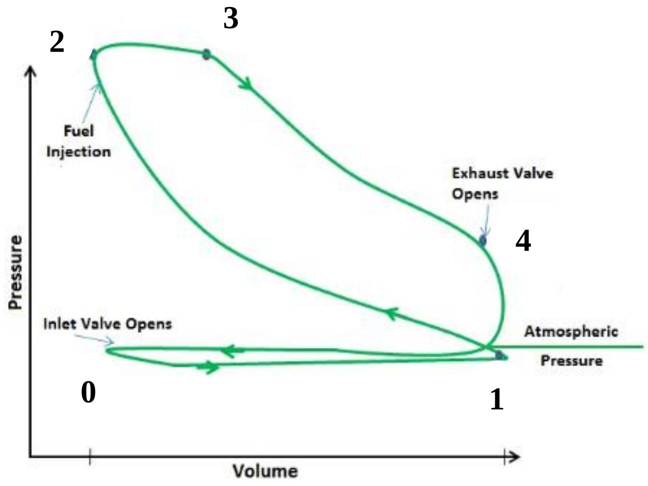
$$W_{34} = \frac{m_m R_p (T_3 - T_4)}{\gamma_p - 1}$$

$$W_{12} = \frac{m_m R_m (T_2 - T_1)}{\gamma_m - 1}$$

$$W_{net} = W_{34} - W_{12}$$

$$\eta_{th} = \frac{w_{net}}{Q_{add}}$$

2-constant pressure cycle (Diesel engine cycle):



Actual p-v Diagram for a Four Stroke Diesel Cycle Engine

$$\boldsymbol{f = \frac{P_{exh}}{P_4} * \frac{1}{r}}$$

$$\dot{\boldsymbol{m}}_{\boldsymbol{m}} = (\dot{\boldsymbol{m}}_{\boldsymbol{air}} + \dot{\boldsymbol{m}}_{\boldsymbol{R}})$$

at point (1) $\boldsymbol{m} = \dot{\boldsymbol{m}}_{\boldsymbol{R}}$

(0-1) intake stroke (air only)

(1-2) compression stroke (air + Residual gases)

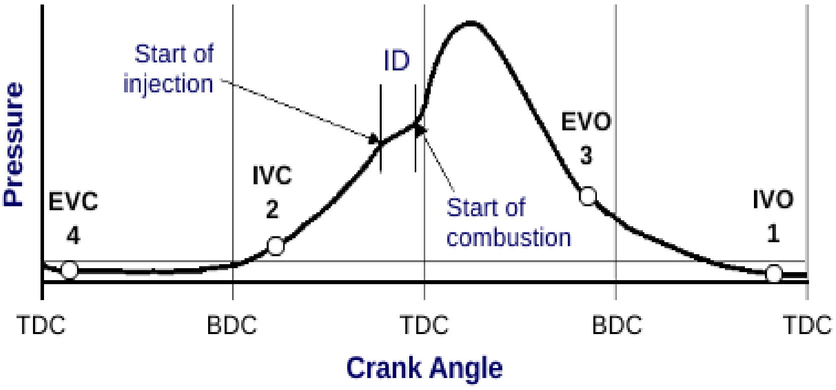
$$\dot{\boldsymbol{m}}_{\boldsymbol{m}} = (\dot{\boldsymbol{m}}_{\boldsymbol{air}} + \dot{\boldsymbol{m}}_{\boldsymbol{R}})$$

$$C_{pm} = \sum \frac{m_i}{m_m} C_{pi}$$

$$C_{pm} = \sum \frac{m_i}{m} C_{pi} = \frac{1}{m_m}(m_{air} C_{pair} + m_R C_{pR})$$

$$C_{Vm} = \sum \frac{m_i}{m} C_{Vi}$$

$$R_m = \sum \frac{m_i}{m} R_i$$



$$Q_{add} = m_m c_{pm}(T_3 - T_2)$$

$$Q_{add} = \dot{m}_f * L.C.V$$

$$W_{34} = \frac{m_m R_p (T_3 - T_4)}{\gamma_p - 1}$$

$$W_{12} = \frac{m_m R_m (T_2 - T_1)}{\gamma_m - 1}$$

$$W_{net} = W_{34} - W_{12}$$

$$\eta_{th} = \frac{w_{net}}{Q_{add}}$$

$$T_3 = T_{max}$$

$$P_3 = P_{max}$$

Prosses 3-4 isentropic expansion

T_4: Temperature of exhaust

P_4: pressure at the end of expansion (before the exhaust valve opened)

Calculation of trapped temperature:

T_1**:** trapped Temperature

Enthalpy balance

1- For constant volume cycle

$$H = \sum H_i \ldots\ldots\ldots\ldots..(A)$$

$$H_m = \left(H_{air} + H_f + H_R\right)$$

$$H_m = m_m C_{Pm}(T_1 - 273) \ldots\ldots\ldots(1)$$

$$H_{air} = m_{air} C_{Pair}(T_{air} - 273) \ldots\ldots\ldots(2)$$

$$H_f = m_f C_{Pf}\left(T_f - 273\right) \ldots\ldots\ldots(3)$$

$$H_R = m_R C_{PR}(T_R - 273) \ldots\ldots\ldots(4)$$

Put equ (1,2,3,4) in equ A

$$m_m C_{Pm}(T_1 - 273) = m_{air} C_{Pair}(T_{air} - 273) + m_f C_{Pf}\left(T_f - 273\right) + m_R C_{PR}(T_R - 273)$$

2- For constant pressure cycle :

$$H = \sum H_i \ldots\ldots\ldots\ldots..(A)$$

$$H_m = (H_{air} + H_R)$$

$$H_m = m_m C_{Pm}(T_1 - 273) \ldots\ldots\ldots(1)$$

$$H_{air} = m_{air} C_{Pair}(T_{air} - 273) \ldots\ldots\ldots(2)$$

$$H_R = m_R C_{PR}(T_R - 273) \ldots\ldots\ldots(3)$$

$$m_m C_{Pm}(T_1 - 273) = m_{air} C_{Pair}(T_{air} - 273) + m_R C_{PR}(T_R - 273)$$

Ex1: a constant volume fuel air cycle of compression ratio (7) uses a fuel of C_8H_{18} .the actual air -fuel ratio is 120% of the stoichiometric one. the ambient Patm is 1.01 bar & Temp is 30ºC. the temperature and pressure before the exhaust valve opened is 1100 K and 5bar. calculate the maximum temperature in the cycle. mean effective pressure and thermal efficiency. taking in the account that for reactants (total charge) m=28.5, cp =1.45 kj/kg.k , L.C.V =40000 kj /kg .assume Tf=20 ºC , Cpf=1.8 kj/kg.k

Sol:

$$C_8H_{18} + A(O_2 + 3.76N_2) \longrightarrow aCO_2 + bH_2O + A * 3.76N_2$$

$$A = n + \frac{m}{4} = 8 + \frac{18}{4} = 5$$

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

$$(\frac{A}{F})_{stoic} = \frac{12.5 * 32 + 12.5 * 3.76 * 28}{[(8 * 12) + (18 * 1)]} = 15$$

$$\left(\frac{A}{F}\right)_{actual} = 1.2 * 15 = 18$$

$$\boldsymbol{F} = \frac{\dot{\boldsymbol{m}}_{\boldsymbol{f}}}{\dot{\boldsymbol{m}}_{\boldsymbol{air}}} = \frac{\mathbf{1}}{\left(\frac{\boldsymbol{A}}{\boldsymbol{F}}\right)} = \frac{1}{18} = 0.0553$$

$$f = \frac{P_{exh}}{P_4} * \frac{1}{r}$$

$$f = \frac{1.01}{5} * \frac{1}{7} = 0.0288$$

$$\dot{m}_{air} = (1-f) = 1 - 0.0288 = 0.971\,kg$$
$$\dot{m}_f = (1-f)F = (1-0.0288)0.0559 = 0.0542\,kg$$
$$\dot{m}_R = (1+F)f = (1+0.0559)0.0288 = 0.0304\,kg$$
$$\dot{m}_m = (1+F) = 1+0.0559 = 1.0559\text{ kg}$$

$$H_m = \left(H_{air} + H_f + H_R\right)$$

$$m_m C_{Pm}(T_1 - 273) = m_{air} C_{Pair}(T_{air} - 273) + m_f C_{Pf}\left(T_f - 273\right) + m_R C_{PR}(T_R - 273)$$

$$1.0559 * 1.45(T_1 - 273) = 0.971 * 1.005(303-273) + 0.0542 * 1.8(293-273) + 0.0304 * 1.15(1100-273) \Rightarrow \mathbf{T_1 = 312.279\ K}$$

$$\gamma_m = \frac{C_{pm}}{C_{Vm}} \qquad C_{Vm} = C_{pm} - R_m$$

$$R_m = \frac{R_0}{M} = \frac{8.314}{28.5} = 0.2918\frac{KJ}{Kg.K}$$

$$C_{Vm} = C_{pm} - R = 1.45 - 0.2918 = 1.16\frac{KJ}{Kg.K}$$

$$\gamma_m = \frac{C_{pm}}{C_{Vm}} = \frac{1.45}{1.16} = 1.25$$

$$T_2 = T_1(r)^{\gamma-1} = 312.279(r)^{1.25-1} = 507.94\,K$$

$$Q_{add} = \dot{m_f} * L.C.V = 0.0542 * 40000 = 2168\,kJ$$

$$Q_{add} = \dot{m_m} C_{Vm}(T_3 - T_2) = 2168 = 1.0559 * 1.16(T_3 - 507.94)$$

$$T_3 = 2277.96K$$

$$mep = \frac{W_{net}}{(V_1 - V_2) * 10^2}$$

$$W_{12}=\frac{m_m R_m (T_2-T_1)}{\gamma_m-1}=\frac{1.0559*0.29(507.94-312.279)}{1.25-1}$$
$$=239.65KJ/Kg$$

$$\gamma_p=\frac{C_{pp}}{C_{Vp}} \qquad C_{Vp}=C_{pp}-R_p$$

$$R=\frac{R_0}{M}=\frac{8.314}{30.5}=0.2725\frac{KJ}{Kg.K}$$

$$C_{Vp}=C_{pp}-R_p=1.15-0.2725=0.877\frac{KJ}{Kg.K}$$

$$\gamma=\frac{C_{pm}}{C_{Vm}}=\frac{1.15}{0.877}=1.31$$

$$W_{34}=\frac{m_m R_p (T_3-T_4)}{\gamma_p-1}=\frac{1.0559*0.2725(2277.96-1100)}{1.31-1}$$
$$=1093.34KJ/Kg$$

$$W_{net}=W_{34}-W_{12}=1093.34-239.65=853.747KJ/Kg$$

$$P_1V_1=m_m R_m T_1$$

$$1.01*V_1=1.0559*0.2918*303$$

$$V_1=0.92\,m^3$$

$$r=\frac{V_1}{V_2}\ \Rightarrow V_2=0.132\,m^3$$

$$mep=\frac{W_{net}}{(V_1-V_2)*10^2}=\frac{853.747}{(0.92-0.132)*10^2}=10.83\,bar$$

$$\eta_{th}=\frac{W_{net}}{Q_{add}}=\frac{853.747}{2168}=39.37\%$$

EX2: A constant pressure fuel-air cycle , the compression ratio is 16 , and the ambient condition are 1.0 bar & 25ºC . the fuel air ratio is gives as 0.075 & residual gas fraction is 5% . if the pressure at the end of expansion stroke is 6 bar and exhaust temperature 1000K and the L.C.V 42000 KJ /Kg .Calculate the cut off ratio and *mep* .assume C_{pR} is 1.2 KJ /Kg.K & *M=29 &* for reactants (total charge) m=28

Sol:

$$\dot{\boldsymbol{m}}_{\boldsymbol{air}} = (1-f) = 1-0.05 = 0.95\,kg$$
$$\dot{\boldsymbol{m}}_{\boldsymbol{R}} = (1+F)f = (1+0.075)0.05 = 0.0537\,kg$$
$$\dot{\boldsymbol{m}}_{\boldsymbol{m}} = (1+F) = 1+0.0559=1.0037 \text{ kg}$$

$$C_{pm} = \sum \frac{m_i}{m} C_{pi} = \frac{1}{1.0037}(0.95 * 1.005 + 0.0537 * 1.2)$$
$$= 1.015\,KJ/Kg.K$$

$$H_m = (H_{air} + H_R)$$

$$m_m C_{Pm}(T_1 - 273) = m_{air} C_{Pair}(T_{air} - 273) + m_R C_{PR}(T_R - 273)$$

$$1.0037 * 1.015(T_1 - 273)$$
$$= 0.95 * 1.005(298 - 273) + 0.0537 * 1.2(1000 - 273)$$
$$\Rightarrow \quad T_1 = 380\,K$$

$$R_m = \frac{R_0}{M} = \frac{8.314}{28} = 0.2969\frac{KJ}{Kg.K}$$
$$C_{Vm} = C_{pm} - R_m = 1.015 - 0.2969 = 0.718$$
$$\gamma_m = \frac{C_{pm}}{C_{Vm}} = \frac{1.015}{0.718} = 1.41$$

$$T_2 = T_1(r)^{\gamma-1} = 380(16)^{1.41-1} = 1184\ K$$

$$\dot{\boldsymbol{m}}_{\boldsymbol{f}} = (1-f)F = (1-0.05)0.075 = 0.0712\ kg$$

$$Q_{add} = \dot{m_f} * L.C.V = 0.0712 * 42000 = 2990\ kJ$$

$$Q_{add} = \dot{m_m} C_{Vm}(T_4 - T_3) = 2990 = 1.0037 * 1.015(T_4 - 1184)$$

$$T_3 = 4119.34K$$

$$mep = \frac{W_{net}}{(V_1 - V_2) * 10^2}$$

$$W_{12} = \frac{m_m R_m (T_2 - T_1)}{\gamma_m - 1} = \frac{1.0037 * 0.2969(1184 - 380)}{1.41 - 1}$$
$$= 584.34KJ/Kg$$

$$\gamma_p = \frac{C_{pp}}{C_{Vp}} \qquad C_{Vp} = C_{pp} - R_p$$

$$R = \frac{R_0}{M} = \frac{8.314}{29} = 0.286 \frac{KJ}{Kg.K}$$

$$C_{Vp} = C_{pp} - R_p = 1.2 - 0.286 = 0.914 \frac{KJ}{Kg.K}$$

$$\gamma_p = \frac{C_{pp}}{C_{Vp}} = \frac{1.2}{0.914} = 1.312$$

$$W_{34} = \frac{m_m R_p (T_3 - T_4)}{\gamma_p - 1} = \frac{1.0037 * 0.286(4119.34 - 1000)}{1.312 - 1}$$
$$= 2869.97KJ/Kg$$

$$W_{net} = W_{34} - W_{12} = 2869.97 - 584.34 = 2285.63KJ/Kg$$

$$P_1 V_1 = m_m R_m T_1$$

$$100 * V_1 = 1.0037 * 0.2969 * 380$$

$$V_1 = 1.132\, m^3$$

$$r = \frac{V_1}{V_2} \Rightarrow V_2 = 0.0707 m^3$$

$$mep = \frac{W_{net}}{(V_1 - V_2) * 10^2} = \frac{2285.63}{(1.132 - 0.0707) * 10^2} = 21.53\, bar$$

$$e = \frac{Vcutoff\ vol}{Vmin} = \frac{V3}{V2}$$

$$\frac{V3}{V2} = \frac{T3}{T2} = \frac{4119.34}{1184} = 3.479$$

Lecture No (10)

HYDROCARBON FUELS

1. Class: third Year

2. Subject: hydrocarbon fuels

3. Number of weeks: Two week

4. Central idea: hydrocarbon fuels

5. The Test:

Hydrocarbon fuels

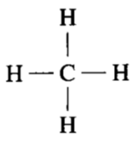
SOME COMMON HYDROCARBON COMPONENTS

Carbon atoms form four bonds in molecular structures, while hydrogen has one bond. A *saturated* hydrocarbon molecule will have no double or triple carbon-to carbon bonds and will have a maximum number of hydrogen atoms. An *unsaturated* molecule will have double or triple carbon-to-carbon bonds. A number of different *families* of hydrocarbon molecules have been identified; a few of the more common ones are described :

Paraffins

The paraffin family (sometimes called alkanes) are chain molecules with a carbon-hydrogen combination of *CnH2n+* 2, *n* being any number. The simplest member of this family, and the simplest of all stable hydrocarbon molecules, is methane(CH4), which is the main component of natural gas. It can be pictured as:

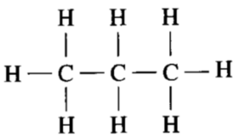
methane (CH_4)



$$\begin{array}{ccccc} & & H & & \\ & & | & & \\ H & - & C & - & H \\ & & | & & \\ & & H & & \end{array}$$

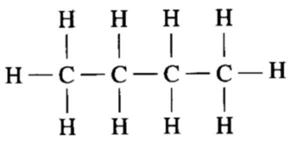
Other species of this family include:

propane (C_3H_8)



$$\begin{array}{ccccccccc} & & H & & H & & H & & \\ & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & H \\ & & | & & | & & | & & \\ & & H & & H & & H & & \end{array}$$

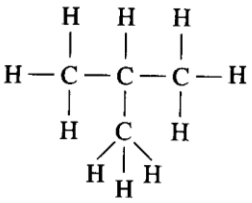
butane (C_4H_{10})



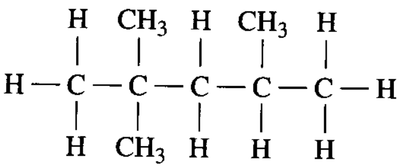
$$\begin{array}{ccccccccccc} & & H & & H & & H & & H & & \\ & & | & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & C & - & H \\ & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & \end{array}$$

Sometimes the chains in the molecule are branched, and other molecular structures are obtained with the same number of carbon and hydrogen atoms. One such *isomer* is isobutane, which has the same chemical formula as butane (C_4H_{10}) but has a different structure:

isobutane (C_4H_{10})



isooctane (C_8H_{18})

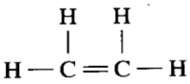


$$\begin{array}{ccccccccccccc} & & H & & CH_3 & & H & & CH_3 & & H & & \\ & & \mid & & \mid & & \mid & & \mid & & \mid & & \\ H & - & C & - & C & - & C & - & C & - & C & - & H \\ & & \mid & & \mid & & \mid & & \mid & & \mid & & \\ & & H & & CH_3 & & H & & H & & H & & \end{array}$$

2 Olefins

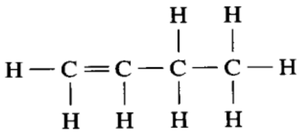
The olefin family consists of chain molecules that contain one double carbon–carbon bond, and are therefore unsaturated. The prefixes from Table 4-2 are used with the suffix "ene." The chemical makeup is C_nH_{2n}. Examples of olefins are:

ethene (C_2H_4)



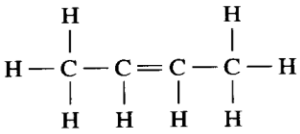
$$\begin{array}{ccccccc} & & H & & H & & \\ & & \mid & & \mid & & \\ H & - & C & = & C & - & H \end{array}$$

butene-1 (C_4H_8)



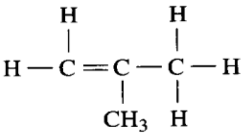
$$\begin{array}{ccccccccccc} & & & & & & H & & H & & \\ & & & & & & \mid & & \mid & & \\ H & - & C & = & C & - & C & - & C & - & H \\ & & \mid & & \mid & & \mid & & \mid & & \\ & & H & & H & & H & & H & & \end{array}$$

butene-2 (C_4H_8)



$$\begin{array}{ccccccccccc} & & H & & & & & & H & & \\ & & \mid & & & & & & \mid & & \\ H & - & C & - & C & = & C & - & C & - & H \\ & & \mid & & \mid & & \mid & & \mid & & \\ & & H & & H & & H & & H & & \end{array}$$

isobutene or 2-methylpropene (C_4H_8)

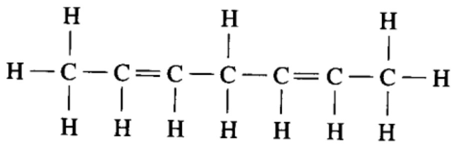


$$\begin{array}{ccccccccc} & & H & & & & H & & \\ & & \mid & & & & \mid & & \\ H & - & C & = & C & - & C & - & H \\ & & & & \mid & & \mid & & \\ & & & & CH_3 & & H & & \end{array}$$

3 Diolefins

Diolefins are chain molecules similar to olefins, except that they have two double carbon–carbon bonds. These unsaturated compounds have the chemical formula C_nH_{2n-2} and use the suffix “diene.”

2,5-heptadiene (C_7H_{12})



$$\begin{array}{ccccccccccccccccc} & & H & & & & & & H & & & & & & H & & \\ & & | & & & & & & | & & & & & & | & & \\ H & - & C & - & C & = & C & - & C & - & C & = & C & - & C & - & H \\ & & | & & | & & | & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & H & & H & & H & & \end{array}$$

4 Acetylene

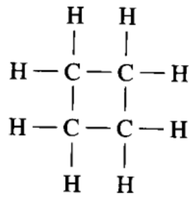
The acetylene family has unsaturated chain molecules with a triple carbon–carbon bond and the chemical formula C_nH_{2n-2}. The best known member of the family is acetylene (C_2H_2).

acetylene (C_2H_2) $H-C\equiv C-H$

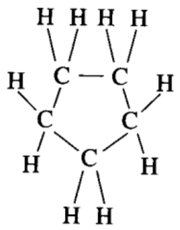
5 Cycloparaffins

Cycloparaffins have unsaturated molecules with a single-bond ring and a chemical formula of C_nH_{2n}.

cyclobutane (C_4H_8)



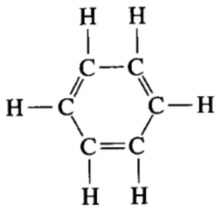
cyclopentane (C_5H_{10})



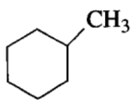
Many variations of these molecules are possible, with one or more of the attached hydrogen atoms replaced with various side radicals and/or chains. Cycloparaffins make good automobile gasoline components.

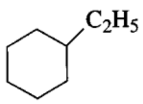
6 Aromatics

Aromatic molecules have an unsaturated ring structure with double carbon–carbon bonds and a general chemical formula of C_nH_{2n-6}. The basic molecule in this family is the benzene ring:

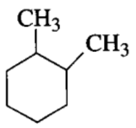

benzene (C_6H_6)

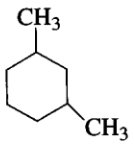
This is modified by replacing the hydrogen atoms with various groups:

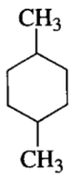

toluene (C_7H_8)


ethylbenzene (C_8H_{10})

When more than one hydrogen atom is replaced, many isomers are possible:

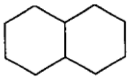

orthoxylene (C_8H_{10})


metaxylene (C_8H_{10})

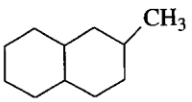

paraxylene (C_8H_{10})

When more than one ring combine in a single large molecule, many additional species are possible:

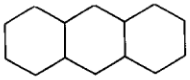
$C_{10}H_8$



$C_{11}H_{10}$



$C_{14}H_{10}$

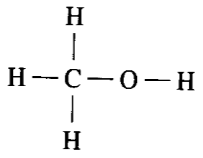


Aromatics generally make good gasoline fuel components, with some exceptions due to exhaust pollution. They have high densities in the liquid state and thus have high energy content per unit volume. Aromatics have high solvency characteristics, and care must be used in material selection for the fuel delivery system (e.g., they will dissolve or swell some gasket materials). Aromatics will dissolve a greater amount of water than some other hydrocarbons and thus can create fuel line freezing problems when the temperature is lowered and some of the water comes out of solution. Aromatics make poor CI engine fuel.

7 Alcohol

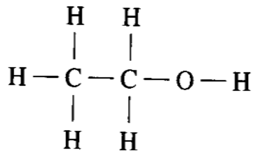
Alcohols are similar to paraffins with one of the hydrogen atoms replaced with the hydroxyl radical OH. The most common alcohols are:

methyl alcohol (methanol), CH_3OH



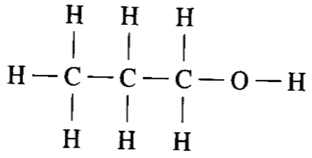
$$H-\overset{H}{\underset{H}{C}}-O-H$$

ethyl alcohol (ethanol), C_2H_5OH



$$H-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-O-H$$

propyl alcohol (propanol), C_3H_7OH



$$H-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-O-H$$

1-Hydrocarbon fuels gasoline

The main fuel for SI engines is gasoline, which is a mixture of many hydrocarbon components and is manufactured from crude petroleum . Crude oil is made up almost entirely of carbon and hydrogen with some traces of other species. It varies from 83% to 87% carbon and 11% to 14% hydrogen by weight The crude oil mixture which is taken from the ground is separated into component products by *cracking* and/or distillation using thermal or catalytic methods at an oil refinery. Cracking is the process of breaking large molecular components into more useful components of smaller molecular weight. Preferential distillation is used to separate the mixtures into single components or smaller ranges of components. Generally, the larger the molecular weight of a component, the higher is its boiling temperature. Low boiling temperature components (smaller molecular weights) are used for solvents and fuels (gasoline), while high boiling temperature components with their large molecular weights are used for tar and asphalt or returned to the refining process for further cracking. The component mixture of the refining process is used for many products, including:

automobile gasoline , diesel fuel , aircraft gasoline ,jet fuel ,home heating fuel ,industrial heating fuel ,natural gas ,lubrication oil , asphalt ,alcohol ,rubber ,paint , plastics , explosives

2-DIESEL FUEL

Diesel fuel (diesel oil, fuel oil) is obtainable over a large range of molecular weights and physical properties. Diesel fuel can be classified as Light diesel fuel has a molecular weight of about 170 and can be approximated by the chemical formula $C_{12.3}H_{22.2}$. Light diesel fuel will be less viscous and easier to pump, will generally inject into smaller droplets, and will be more costly. Heavy diesel fuel has a molecular weight of about 200 and can be approximated as $C_{14.6}H_{24.8}$.. Heavy diesel fuel can generally be used in larger engines with higher injection pressures and heated intake systems. Often an automobile or light truck can use a less costly heavier fuel in the summer, but must change to a lighter, less viscous fuel in cold weather because of cold starting and fuel line pumping problems.

ALTERNATE FUELS

1-Alcohol

Alcohols are an attractive alternate fuel because they can be obtained from a number of sources, both natural and manufactured. Methanol (methyl alcohol) and ethanol (ethyl alcohol) are two kinds of alcohol that seem most promising and have had the most development as engine fuel.

The advantages of alcohol as a fuel include:

1. Can be obtained from a number of sources, both natural and manufactured.

2. Is high octane fuel with anti-knock index numbers (octane number on fuel

pump) of over 100. High octane numbers result, at least in part, from the high flame speed of alcohol. Engines using high-octane fuel can run more efficiently by using higher compression ratios.

3. Generally less overall emissions when compared with gasoline.

4. When burned, it forms more moles of exhaust, which gives higher pressure and more power in the expansion stroke.

5. Has high evaporative cooling *(hfg)* which results in a cooler intake process and compression stroke. This raises the volumetric efficiency of the engine and reduces the required work input in the compression stroke.

6. Low sulfur content in the fuel.

The disadvantages of alcohol fuels include:

1. Low energy content of the fuel. This means that almost twice as much alcohol as gasoline must be burned to give the same energy input to the engine. With equal thermal efficiency and similar engine output usage, twice as much fuel would have to be purchased, and the distance which could be driven with a given fuel tank volume would be cut in half. The same amount of automobile use would require twice as much storage capacity in the distribution system, twice the number of storage facilities, twice the volume of storage at the service station, twice as many tank trucks and pipelines, etc. Even with the lower energy content of alcohol, engine power for a given displacement would be about the same. This is because of the lower air-fuel ratio needed by alcohol. Alcohol contains oxygen and thus requires less air for stoichiometric combustion. More fuel can be burned with the same amount of air.

2. More aldehydes in the exhaust. If as much alcohol fuel was consumed as gasoline, aldehyde emissions would be a serious exhaust pollution problem.

3. Alcohol is much more corrosive than gasoline on copper, brass, aluminum, rubber, and many plastics. This puts some restrictions on the design and manufacturing of engines to be used with this fuel. This should also be considered when alcohol fuels are used in engine systems designed to be used with gasoline. Fuel lines and tanks, gaskets, and even metal engine parts can deteriorate with long-term alcohol use (resulting in cracked fuel lines, the need for special fuel tank, etc). Methanol is very corrosive on metals.

4. Poor cold weather starting characteristics due to low vapor pressure and evaporation. Alcohol-fueled engines generally have difficulty starting at temperatures below 10°C. Often a small amount of gasoline is added to alcohol fuel, which greatly improves cold-weather starting. The need to do this, however, greatly reduces the attractiveness of any alternate fuel.

5. Poor ignition characteristics in general.

6. Alcohols have almost invisible flames, which is considered dangerous when
handling fuel. Again, a small amount of gasoline removes this danger.

7. Danger of storage tank flammability due to low vapor pressure. Air can leak into storage tanks and create a combustible mixture.

8. Low flame temperatures generate less NOx, but the resulting lower exhaust temperatures take longer to heat the catalytic converter to an efficient operating temperature.

9. Many people find the strong odor of alcohol very offensive. Headaches and dizziness have been experienced when refueling an automobile.

10. Vapor lock in fuel delivery systems

2-Hydrogen

advantages of using hydrogen as a fuel:

1. Low emissions. Essentially no CO or HC in the exhaust as there is no carbon in the fuel. Most exhaust would be H20 and N2•

2. Fuel availability. There are a number of different ways of making hydrogen, including electrolysis of water.

3. Fuel leakage to environment is not a pollutant.

4. High energy content per volume when stored as a liquid. This would give a large vehicle range for a given fuel tank capacity, but see the following.

Disadvantages of using hydrogen as a fuel:

1. Heavy, bulky fuel storage, both in vehicle and at the service station. Hydrogen can be stored either as a cryogenic liquid or as a compressed gas. If stored as a liquid, it would have to be kept under pressure at a very low temperature. This would require a thermally super-insulated fuel tank. Storing in a gas phase would require a heavy pressure vessel with limited capacity.

2. Difficult to refuel.

3. Poor engine volumetric efficiency. Any time a gaseous fuel is used in an engine,

the fuel will displace some of the inlet air and poorer volumetric efficiency will result.

4. Fuel cost would be high at present-day technology and availability.
5. High NOx emissions because of high flame temperature.
6. Can detonate.

3-Natural Gas-Methane

Natural gas is a mixture of components, consisting mainly of methane (60-98%) with small amounts of other hydrocarbon fuel components. In addition it contains various amounts of N2, CO2, He, and traces of other gases. Its sulfur content ranges from very little (sweet) to larger amounts (sour). It is stored as compressed natural gas (CNG) at pressures of 16 to 25 MPa, or as liquid natural gas (LNG) at pressures of 70 to 210 kPa and a temperature around -160°C. As a fuel, it works best in an engine system with a single-throttle body fuel injector. This gives a longer mixing time, which is needed by this fuel. Tests using CNG in various sized vehicles continue to be conducted by government agencies and private industry

Advantages of natural gas as a fuel include:

1. Octane number of 120, which makes it a very good SI engine fuel. One reason for this high octane number is a fast flame speed. Engines can operate with a high compression ratio.
2. Low engine emissions. Less aldehydes than with methanol.
3. Fuel is fairly abundant worldwide with much available in the United States. It can be made from coal but this would make it more costly.

Disadvantages of natural gas as an engine fuel:

1. Low energy density resulting in low engine performance.
2. Low engine volumetric efficiency because it is a gaseous fuel.
3. Need for large pressurized fuel storage tank. Most test vehicles have a range of only about 120 miles. There is some safety concern with a pressurized fuel tank.
4. Inconsistent fuel properties.
5. Refueling is slow process.

4- Propane

Propane has been tested in fleet vehicles for a number of years. It is a good high octane SI engine fuel and produces less emissions than gasoline: about 60% less CO, 30% less HC, and 20% less NOx. Propane is stored as a liquid under pressure and delivered through a high-pressure line to the engine, where it is vaporized. Being a gaseous fuel, it has the disadvantage of lower engine volumetric efficiency

And other type of fuel

5- **Reformulated Gasoline**.

6- **Coal-Water Slurry**

Lecture No (11)

Octane Number &Cetane Number

1. Class: third Year

2. Subject: Octane Number &Cetane Number

3. Number of weeks: one week

4. Central idea: Octane Number &Cetane Number

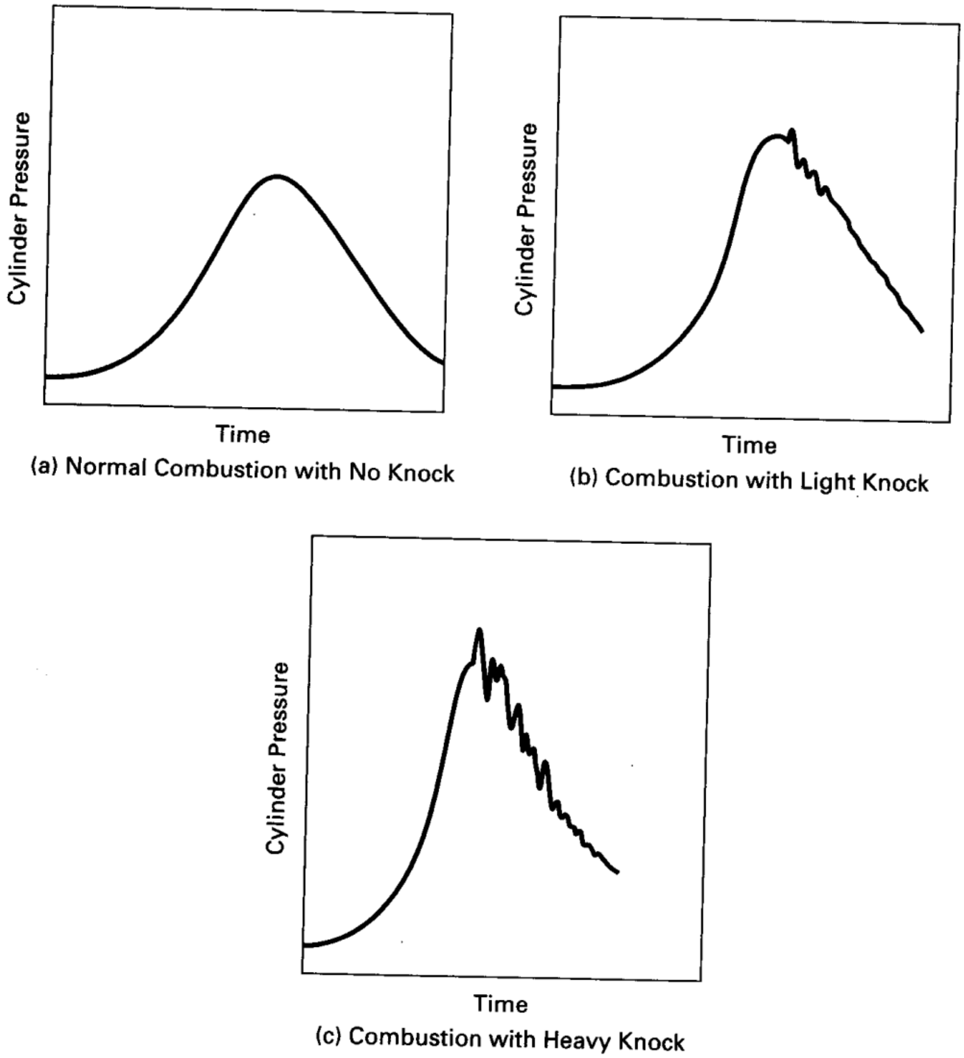
5. The Test:

Octane Number &Cetane Number

Self-Ignition Characteristics of Fuels

If the temperature of an air-fuel mixture is raised high enough, the mixture will self ignite without the need of a spark plug or other external igniter. The temperature above which this occurs is called the **self-ignition temperature** (SIT). This is the basic principle of ignition in a compression ignition engine. The compression ratio is high enough so that the temperature rises above SIT during the compression stroke. Self ignition then occurs when fuel is injected into the combustion chamber. On the other hand, self-ignition (or pre-ignition, or auto-ignition) is not desirable in an SI engine, where a spark plug is used to ignite the air-fuel at the proper time in the cycle. The compression ratios of gasoline-fueled SI engines are limited to about 11:1 to avoid self-ignition. When self-ignition does occur in an SI engine higher than desirable, pressure pulses are generated. These high-pressure pulses can cause damage to the engine and quite often are in the audible frequency range. This phenomenon is often called knock or ping.

Figure **(1)** shows the pressure-time history within a cylinder of a typical SI engine. With no self-ignition the pressure force on the piston follows a smooth curve, resulting in smooth engine operation. When self-ignition does occur, pressure forces on the piston are not smooth and engine knock occurs



(a) Normal Combustion with No Knock

(b) Combustion with Light Knock

(c) Combustion with Heavy Knock

Figure 1 Cylinder pressure as a function of time in a typical SI engine combustion chamber showing **(a)** normal combustion, **(b)** combustion with light knock, and **(c)** combustion with heavy knock. Adapted from [33].

The idea of combustion can then be extrapolated to real combustion engine shapes. Before combustion the chamber is divided into four equal mass units, each occupying an equal volume. Combustion starts at the spark plug on the left side, and the flame front travels from left to right. As combustion occurs, the temperature of the burned gases is increased to a high value. This, in turn, raises the pressure of the burned gases and expands the volume of that mass as shown in Fig. 2(b). The unburned gases in front of the flame front are compressed by this higher pressure, and compressive heating raises the temperature of the gas. The temperature of the unburned gas is further raised by radiation heating from the flame, and this then raises the pressure even higher. Heat transfer by conduction and convection are not important during this process due to the very short time interval involved.

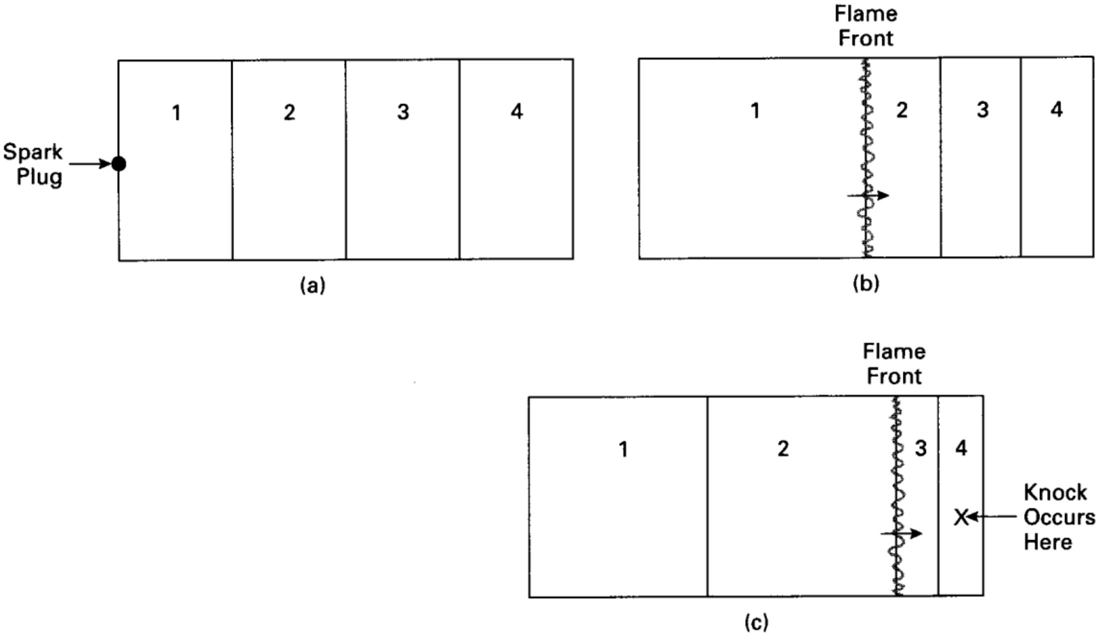
The flame front moving through the second mass of air-fuel does so at an accelerated rate because of the higher temperature and pressure, which increase the reaction rate. This, in turn, further compresses and heats the unburned gases in front of the flame as shown in Fig. 4-5(c). In addition, the energy release in the combustion process raises further the temperature and pressure of the burned gases behind the flame front. This occurs both by compressive heating and radiation. Thus, the flame front continues its travel through an unburned mixture that is progressively higher in temperature and pressure. By the time the flame reaches the last portion of unburned gas, this gas is at a very high temperature and pressure. In this *end gas* near the end of the combustion process is where self-ignition and knock occur.

To avoid knock, it is necessary for the flame to pass through and consume all unburned gases which have risen above self-ignition temperature before the ignition delay time elapses. This is done by

1-a combination of fuel property control

2-design of combustion chamber geometry.

. By limiting the compression ratio in an SI engine, the temperature at the end of the compression stroke where combustion starts is limited. The reduced temperature at the start of combustion then reduces the temperature throughout the entire combustion process, and knock is avoided. On the other hand, a high compression ratio will result in a higher temperature at the start of combustion.



(a) (b)

(c)

Octane Number and Engine Knock

The fuel property that describes how well a fuel will or will not self-ignite is called the octane number or just octane.

The two standard reference fuels used are

1- Isooctane = octane number (ON) of 100 .(high-compression ratios)
2- n-heptane =octane number (ON) of 0 (low compression ratios)

There are several different tests used for rating octane numbers,

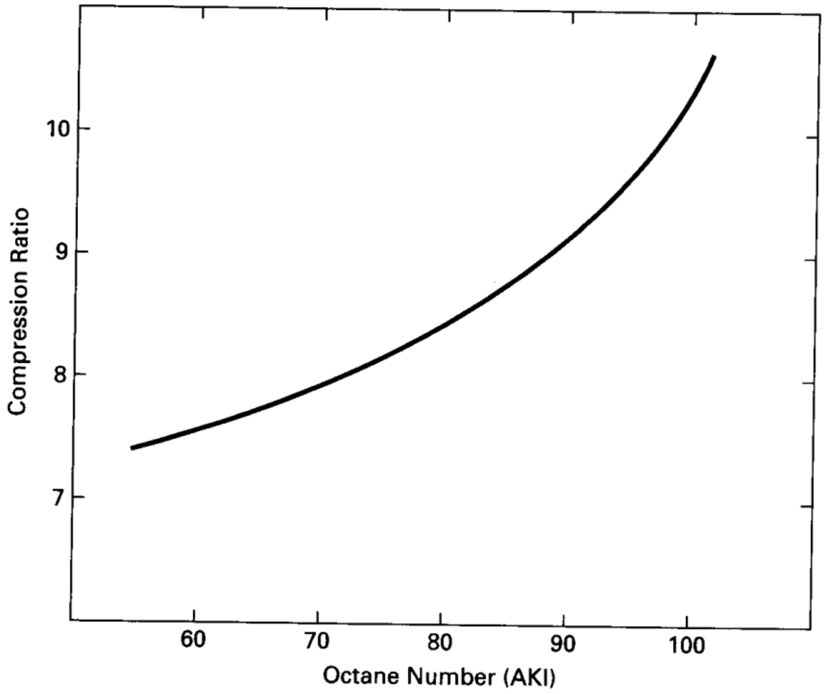
1- Motor Method (MON)
2- Research Method (RON)
3-anti-knock index: AKI = (MON + *RON)/2*

Common octane numbers (anti-knock index) for gasoline fuels used in automobiles range from 87 to 95, with higher values available for special high-performance and racing engines. Reciprocating SI aircraft engines usually use low-lead fuels with octane numbers in the 85 to 100 range.

The octane number of a fuel depends on a number of variables, that affect **ON** are combustion chamber geometry, turbulence, swirl, temperature, inert gases, etc.

The higher the flame speed in an air-fuel mixture, the higher the octane number. This is because, with a higher flame speed, the air-fuel mixture that is heated above SIT will be consumed during ignition delay time, and knock will be avoided.

Generally there is a high correlation between the compression ratio and the ON of the fuel an engine requires to avoid knock (Fig. 3).

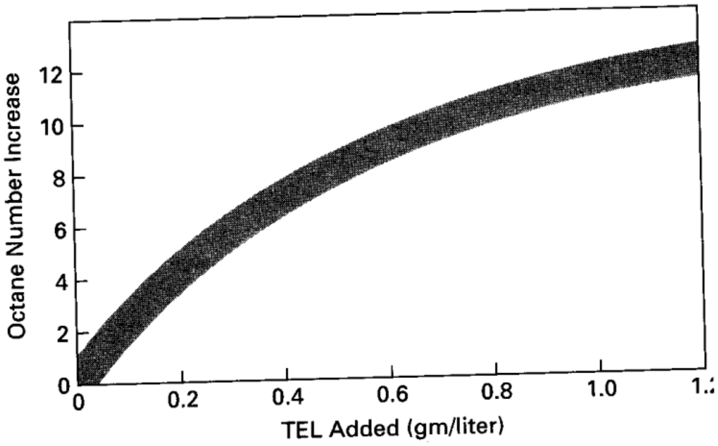


If several fuels of known ON are mixed, a good approximation of the mixture octane number is:

$ON_{mix} = (\% \, of A)(ON_A) + (\% \, of B)(ON_B) + (\% \text{ of } C)(ON_c)$

where % = mass percent.

There are a number of gasoline additives that are used to raise the octane number. For many years the standard additive was tetraethyllead TEL, (C2Hs)4Pb.A few milliliters of TEL in several liters of gasoline could raise the ON several points in a very predictable manner but TEL which has toxic vapors and is even harmful in contact with human skin. (Fig. 4).



Cetane Number

In a compression ignition engine, self-ignition of the air-fuel mixture is a necessity. The correct fuel must be chosen which will self-ignite at the precise proper time in the engine cycle. It is therefore necessary to have knowledge and control of the ignition delay time of the fuel. The property that quantifies this is called the cetane number. The larger the cetane number, the shorter is the ID and the quicker the fuel will self-ignite in the combustion chamber environment. A low cetane number means the fuel will have a long ID. Like octane number rating, cetane numbers are established by comparing the test fuel to two standard reference fuels. The fuel component n-cetane (hexadecane), $C_{16}H_{34}$, is given the cetane number value of 100, while heptamethylnonane (HMN), $C_{12}H_{34}$,is given the value of 15. The cetane number (CN) of other fuels is then obtained by comparing the ID of that fuel to the ID of a mixture blend of the two reference fuels with

CN of fuel = (percent of n-cetane) + (0.15)(percent of HMN)

Normal cetane number range is about 40 to 60. For a given engine injection timing and rate, if the cetane number of the fuel is low the ID will be too long. When this occurs, more fuel than, desirable will be injected into the cylinder before the first fuel particles ignite, causing a very large, fast pressure rise at the start of combustion. This results in low thermal efficiency and a rough-running engine. If the CN

of the fuel is high, combustion will start too soon in the cycle. Pressure will rise before TDC, and more work will be required in the compression stroke.

Cetane numbers below 40 result in unacceptable levels of exhaust smoke and are illegal by many emission laws. The cetane number of a fuel can be raised with certain additives which include nitrates and nitrites. There is a strong inverse correlation between the cetane number of a fuel and its octane number.

APPENDIX

A

SELECTED THERMODYNAMIC PROPERTIES OF GASES COMPRISING C–H–O–N SYSTEM

TABLES A.1 TO A.12

Ideal-gas values for standard reference state ($T = 298.15\,\mathrm{K}$, $P = 1\,\mathrm{atm}$) for

$$\bar{c}_p(T), \bar{h}^o(T) - \bar{h}^o_{f,\mathrm{ref}}, \bar{h}^o_f(T), \bar{s}^o(T), \bar{g}^o_f(T) \qquad \text{for}$$

$$CO, CO_2, H_2, H, OH, H_2O, N_2, N, NO, NO_2, O_2, O.$$

Enthalpy of formation and Gibbs function of formation for compounds are calculated from the elements as

$$\bar{h}^o_{f,i}(T) = \bar{h}^o_i(T) - \sum_{j\,\text{elements}} \nu'_j \bar{h}^o_j(T)$$

$$\bar{g}^o_{f,i}(T) = \bar{g}^o_i(T) - \sum_{j\,\text{elements}} \nu'_j \bar{g}^o_j(T)$$

$$= \bar{h}^o_{f,i}(T) - T\bar{s}^o_i(T) - \sum_{j\,\text{elements}} \nu'_j[-T\bar{s}^o_j(T)].$$

SOURCE: Tables were generated from curvefit coefficients given in Kee, R. J., Rupley, F. M., and Miller, J. A., "The Chemkin Thermodynamic Data Base," Sandia Report, SAND87-8215B, March 1991.

TABLE A.13

Curvefit coefficients for $\bar{c}_p(T)$ for the same gases as above.

SOURCE: ibid.

Table A.1 Carbon monoxide (CO), MW = 28.010, enthalpy of formation @ 298 K (kJ/kmol) = −110, 541

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T)-\bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	28.687	−2,835	−111,308	186.018	−128,532
298	29.072	0	−110,541	197.548	−137,163
300	29.078	54	−110,530	197.728	−137,328
400	29.433	2,979	−110,121	206.141	−146,332
500	29.857	5,943	−110,017	212.752	−155,403
600	30.407	8,955	−110,156	218.242	−164,470
700	31.089	12,029	−110,477	222.979	−173,499
800	31.860	15,176	−110,924	227.180	−182,473
900	32.629	18,401	−111,450	230.978	−191,386
1,000	33.255	21,697	−112,022	234.450	−200,238
1,100	33.725	25,046	−112,619	237.642	−209,030
1,200	34.148	28,440	−113,240	240.595	−217,768
1,300	34.530	31,874	−113,881	243.344	−226,453
1,400	34.872	35,345	−114,543	245.915	−235,087
1,500	35.178	38,847	−115,225	248.332	−243,674
1,600	35.451	42,379	−115,925	250.611	−252,214
1,700	35.694	45,937	−116,644	252.768	−260,711
1,800	35.910	49,517	−117,380	254.814	−269,164
1,900	36.101	53,118	−118,132	256.761	−277,576
2,000	36.271	56,737	−118,902	258.617	−285,948
2,100	36.421	60,371	−119,687	260.391	−294,281
2,200	36.553	64,020	−120,488	262.088	−302,576
2,300	36.670	67,682	−121,305	263.715	−310,835
2,400	36.774	71,354	−122,137	265.278	−319,057
2,500	36.867	75,036	−122,984	266.781	−327,245
2,600	36.950	78,727	−123,847	268.229	−335,399
2,700	37.025	82,426	−124,724	269.625	−343,519
2,800	37.093	86,132	−125,616	270.973	−351,606
2,900	37.155	89,844	−126,523	272.275	−359,661
3,000	37.213	93,562	−127,446	273.536	−367,684
3,100	37.268	97,287	−128,383	274.757	−375,677
3,200	37.321	101,016	−129,335	275.941	−383,639
3,300	37.372	104,751	−130,303	277.090	−391,571
3,400	37.422	108,490	−131,285	278.207	−399,474
3,500	37.471	112,235	−132,283	279.292	−407,347
3,600	37.521	115,985	−133,295	280.349	−415,192
3,700	37.570	119,739	−134,323	281.377	−423,008
3,800	37.619	123,499	−135,366	282.380	−430,796
3,900	37.667	127,263	−136,424	283.358	−438,557
4,000	37.716	131,032	−137,497	284.312	−446,291
4,100	37.764	134,806	−138,585	285.244	−453,997
4,200	37.810	138,585	−139,687	286.154	−461,677
4,300	37.855	142,368	−140,804	287.045	−469,330
4,400	37.897	146,156	−141,935	287.915	−476,957
4,500	37.936	149,948	−143,079	288.768	−484,558
4,600	37.970	153,743	−144,236	289.602	−492,134
4,700	37.998	157,541	−145,407	290.419	−499,684

Table A.1 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	38.019	161,342	−146,589	291.219	−507,210
4,900	38.031	165,145	−147,783	292.003	−514,710
5,000	38.033	168,948	−148,987	292.771	−522,186

Table A.2 Carbon dioxide (CO_2), MW = 44.011, enthalpy of formation @ 298 K (kJ/kmol) = −393,546

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	32.387	−3,423	−393,483	199.876	−394,126
298	37.198	0	−393,546	213.736	−394,428
300	37.280	69	−393,547	213.966	−394,433
400	41.276	4,003	−393,617	225.257	−394,718
500	44.569	8,301	−393,712	234.833	−394,983
600	47.313	12,899	−393,844	243.209	−395,226
700	49.617	17,749	−394,013	250.680	−395,443
800	51.550	22,810	−394,213	257.436	−395,635
900	53.136	28,047	−394,433	263.603	−395,799
1,000	54.360	33,425	−394,659	269.268	−395,939
1,100	55.333	38,911	−394,875	274.495	−396,056
1,200	56.205	44,488	−395,083	279.348	−396,155
1,300	56.984	50,149	−395,287	283.878	−396,236
1,400	57.677	55,882	−395,488	288.127	−396,301
1,500	58.292	61,681	−395,691	292.128	−396,352
1,600	58.836	67,538	−395,897	295.908	−396,389
1,700	59.316	73,446	−396,110	299.489	−396,414
1,800	59.738	79,399	−396,332	302.892	−396,425
1,900	60.108	85,392	−396,564	306.132	−396,424
2,000	60.433	91,420	−396,808	309.223	−396,410
2,100	60.717	97,477	−397,065	312.179	−396,384
2,200	60.966	103,562	−397,338	315.009	−396,346
2,300	61.185	109,670	−397,626	317.724	−396,294
2,400	61.378	115,798	−397,931	320.333	−396,230
2,500	61.548	121,944	−398,253	322.842	−396,152
2,600	61.701	128,107	−398,594	325.259	−396,061
2,700	61.839	134,284	−398,952	327.590	−395,957
2,800	61.965	140,474	−399,329	329.841	−395,840
2,900	62.083	146,677	−399,725	332.018	−395,708
3,000	62.194	152,891	−400,140	334.124	−395,562
3,100	62.301	159,116	−400,573	336.165	−395,403
3,200	62.406	165,351	−401,025	338.145	−395,229
3,300	62.510	171,597	−401,495	340.067	−395,041
3,400	62.614	177,853	−401,983	341.935	−394,838
3,500	62.718	184,120	−402,489	343.751	−394,620
3,600	62.825	190,397	−403,013	345.519	−394,388
3,700	62.932	196,685	−403,553	347.242	−394,141
3,800	63.041	202,983	−404,110	348.922	−393,879
3,900	63.151	209,293	−404,684	350.561	−393,602
4,000	63.261	215,613	−405,273	353.161	−393,311
4,100	63.369	221,945	−405,878	353.725	−393,004
4,200	63.474	228,287	−406,499	355.253	−392,683
4,300	63.575	234,640	−407,135	356.748	−392,346
4,400	63.669	241,002	−407,785	358.210	−391,995
4,500	63.753	247,373	−408,451	359.642	−391,629
4,600	63.825	253,752	−409,132	361.044	−391,247
4,700	63.881	260,138	−409,828	362.417	−390,851

Table A.2 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	63.918	266,528	−410,539	363.763	−390,440
4,900	63.932	272,920	−411,267	365.081	−390,014
5,000	63.919	279,313	−412,010	366.372	−389,572

Table A.3 Hydrogen (H_2), MW = 2.016, enthalpy of formation @ 298 K (kJ/kmol) = 0

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	28.522	−2,818	0	119.137	0
298	28.871	0	0	130.595	0
300	28.877	53	0	130.773	0
400	29.120	2,954	0	139.116	0
500	29.275	5,874	0	145.632	0
600	29.375	8,807	0	150.979	0
700	29.461	11,749	0	155.514	0
800	29.581	14,701	0	159.455	0
900	29.792	17,668	0	162.950	0
1,000	30.160	20,664	0	166.106	0
1,100	30.625	23,704	0	169.003	0
1,200	31.077	26,789	0	171.687	0
1,300	31.516	29,919	0	174.192	0
1,400	31.943	33,092	0	176.543	0
1,500	32.356	36,307	0	178.761	0
1,600	32.758	39,562	0	180.862	0
1,700	33.146	42,858	0	182.860	0
1,800	33.522	46,191	0	184.765	0
1,900	33.885	49,562	0	186.587	0
2,000	34.236	52,968	0	188.334	0
2,100	34.575	56,408	0	190.013	0
2,200	34.901	59,882	0	191.629	0
2,300	35.216	63,388	0	193.187	0
2,400	35.519	66,925	0	194.692	0
2,500	35.811	70,492	0	196.148	0
2,600	36.091	74,087	0	197.558	0
2,700	36.361	77,710	0	198.926	0
2,800	36.621	81,359	0	200.253	0
2,900	36.871	85,033	0	201.542	0
3,000	37.112	88,733	0	202.796	0
3,100	37.343	92,455	0	204.017	0
3,200	37.566	96,201	0	205.206	0
3,300	37.781	99,968	0	206.365	0
3,400	37.989	103,757	0	207.496	0
3,500	38.190	107,566	0	208.600	0
3,600	38.385	111,395	0	209.679	0
3,700	38.574	115,243	0	210.733	0
3,800	38.759	119,109	0	211.764	0
3,900	38.939	122,994	0	212.774	0
4,000	39.116	126,897	0	213.762	0
4,100	39.291	130,817	0	214.730	0
4,200	39.464	134,755	0	215.679	0
4,300	39.636	138,710	0	216.609	0
4,400	39.808	142,682	0	217.522	0
4,500	39.981	146,672	0	218.419	0
4,600	40.156	150,679	0	219.300	0
4,700	40.334	154,703	0	220.165	0

Table A.3 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	40.516	158,746	0	221.016	0
4,900	40.702	162,806	0	221.853	0
5,000	40.895	166,886	0	222.678	0

Table A.4 Hydrogen atom (H), MW = 1.008, enthalpy of formation @ 298 K (kJ/kmol) = 217,977

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	20.786	−2,040	217,346	106.305	207,999
298	20.786	0	217,977	114.605	203,276
300	20.786	38	217,989	114.733	203,185
400	20.786	2,117	218,617	120.713	198,155
500	20.786	4,196	219,236	125.351	192,968
600	20.786	6,274	219,848	129.351	187,657
700	20.786	8,353	220,456	132.345	182,244
800	20.786	10,431	221,059	135.121	176,744
900	20.786	12,510	221,653	137.569	171,169
1,000	20.786	14,589	222,234	139.759	165,528
1,100	20.786	16,667	222,793	141.740	159,830
1,200	20.786	18,746	223,329	143.549	154,082
1,300	20.786	20,824	223,843	145.213	148,291
1,400	20.786	22,903	224,335	146.753	142,461
1,500	20.786	24,982	224,806	148.187	136,596
1,600	20.786	27,060	225,256	149.528	130,700
1,700	20.786	29,139	225,687	150.789	124,777
1,800	20.786	31,217	226,099	151.977	118,830
1,900	20.786	33,296	226,493	153.101	112,859
2,000	20.786	35,375	226,868	154.167	106,869
2,100	20.786	37,453	227,226	155.181	100,860
2,200	20.786	39,532	227,568	156.148	94,834
2,300	20.786	41,610	227,894	157.072	88,794
2,400	20.786	43,689	228,204	157.956	82,739
2,500	20.786	45,768	228,499	158.805	76,672
2,600	20.786	47,846	228,780	159.620	70,593
2,700	20.786	49,925	229,047	160.405	64,504
2,800	20.786	52,003	229,301	161.161	58,405
2,900	20.786	54,082	229,543	161.890	52,298
3,000	20.786	56,161	229,772	162.595	46,182
3,100	20.786	58,239	229,989	163.276	40,058
3,200	20.786	60,318	230,195	163.936	33,928
3,300	20.786	62,396	230,390	164.576	27,792
3,400	20.786	64,475	230,574	165.196	21,650
3,500	20.786	66,554	230,748	165.799	15,502
3,600	20.786	68,632	230,912	166.954	9,350
3,700	20.786	70,711	231,067	166.954	3,194
3,800	20.786	72,789	231,212	167.508	−2,967
3,900	20.786	74,868	231,348	168.048	−9,132
4,000	20.786	76,947	231,475	168.575	−15,299
4,100	20.786	79,025	231,594	169.088	−21,470
4,200	20.786	81,104	231,704	169.589	−27,644
4,300	20.786	83,182	231,805	170.078	−33,820
4,400	20.786	85,261	231,897	170.556	−39,998
4,500	20.786	87,340	231,981	171.023	−46,179
4,600	20.786	89,418	232,056	171.480	−52,361
4,700	20.786	91,497	232,123	171.927	−58,545

Table A.4 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
4,800	20.786	93,575	232,180	172.364	−64,730
4,900	20.786	95,654	232,228	172.793	−70,916
5,000	20.786	97,733	232,267	173.213	−77,103

Table A.5 Hydroxyl (OH), MW = 17.007, enthalpy of formation @ 298 K (kJ/kmol) = 38,985

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	30.140	−2,948	38,864	171.607	35,808
298	29.932	0	38,985	183.604	34,279
300	29.928	55	38,987	183.789	34,250
400	29.718	3,037	39,030	192.369	32,662
500	29.570	6,001	39,000	198.983	31,072
600	29.527	8,955	38,909	204.369	29,494
700	29.615	11,911	38,770	208.925	27,935
800	29.844	14,883	38,599	212.893	26,399
900	30.208	17,884	38,410	216.428	24,885
1,000	30.682	20,928	38,220	219.635	23,392
1,100	31.186	24,022	38,039	222.583	21,918
1,200	31.662	27,164	37,867	225.317	20,460
1,300	32.114	30,353	37,704	227.869	19,017
1,400	32.540	33,586	37,548	230.265	17,585
1,500	32.943	36,860	37,397	232.524	16,164
1,600	33.323	40,174	37,252	234.662	14,753
1,700	33.682	43,524	37,109	236.693	13,352
1,800	34.019	46,910	36,969	238.628	11,958
1,900	34.337	50,328	36,831	240.476	10,573
2,000	34.635	53,776	36,693	242.245	9,194
2,100	34.915	57,254	36,555	243.942	7,823
2,200	35.178	60,759	36,416	245.572	6,458
2,300	35.425	64,289	36,276	247.141	5,099
2,400	35.656	67,843	36,133	248.654	3,746
2,500	35.872	71,420	35,986	250.114	2,400
2,600	36.074	75,017	35,836	251.525	1,060
2,700	36.263	78,634	35,682	252.890	−275
2,800	36.439	82,269	35,524	254.212	−1,604
2,900	36.604	85,922	35,360	255.493	−2,927
3,000	36.759	89,590	35,191	256.737	−4,245
3,100	36.903	93,273	35,016	257.945	−5,556
3,200	37.039	96,970	34,835	259.118	−6,862
3,300	37.166	100,681	34,648	260.260	−8,162
3,400	37.285	104,403	34,454	261.371	−9,457
3,500	37.398	108,137	34,253	262.454	−10,745
3,600	37.504	111,882	34,046	263.509	−12,028
3,700	37.605	115,638	33,831	264.538	−13,305
3,800	37.701	119,403	33,610	265.542	−14,576
3,900	37.793	123,178	33,381	266.522	−15,841
4,000	37.882	126,962	33,146	267.480	−17,100
4,100	37.968	130,754	32,903	268.417	−18,353
4,200	38.052	134,555	32,654	269.333	−19,600
4,300	38.135	138,365	32,397	270.229	−20,841
4,400	38.217	142,182	32,134	271.107	−22,076
4,500	38.300	146,008	31,864	271.967	−23,306
4,600	38.382	149,842	31,588	272.809	−24,528
4,700	38.466	153,685	31,305	273.636	−25,745

Table A.5 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	38.552	157,536	31,017	274.446	−26,956
4,900	38.640	161,395	30,722	275.242	−28,161
5,000	38.732	165,264	30,422	276.024	−29,360

Table A.6 Water (H_2O), MW = 18.016, enthalpy of formation @ 298 K (kJ/kmol) = −241,845, enthalpy of vaporization (kJ/kmol) = 44,010

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	32.255	−3,227	−240,838	175.602	−232,779
298	33.448	0	−241,845	188.715	−228,608
300	33.468	62	−241,865	188.922	−228,526
400	34.437	3,458	−242,858	198.686	−223,929
500	35.337	6,947	−243,822	206.467	−219,085
600	36.288	10,528	−244,753	212.992	−214,049
700	37.364	14,209	−245,638	218.665	−208,861
800	38.587	18,005	−246,461	223.733	−203,550
900	39.930	21,930	−247,209	228.354	−198,141
1,000	41.315	25,993	−247,879	232.633	−192,652
1,100	42.638	30,191	−248,475	236.634	−187,100
1,200	43.874	34,518	−249,005	240.397	−181,497
1,300	45.027	38,963	−249,477	243.955	−175,852
1,400	46.102	43,520	−249,895	247.332	−170,172
1,500	47.103	48,181	−250,267	250.547	−164,464
1,600	48.035	52,939	−250,597	253.617	−158,733
1,700	48.901	57,786	−250,890	256.556	−152,983
1,800	49.705	62,717	−251,151	259.374	−147,216
1,900	50.451	67,725	−251,384	262.081	−141,435
2,000	51.143	72,805	−251,594	264.687	−135,643
2,100	51.784	77,952	−251,783	267.198	−129,841
2,200	52.378	83,160	−251,955	269.621	−124,030
2,300	52.927	88,426	−252,113	271.961	−118,211
2,400	53.435	93,744	−252,261	274.225	−112,386
2,500	53.905	99,112	−252,399	276.416	−106,555
2,600	54.340	104,524	−252,532	278.539	−100,719
2,700	54.742	109,979	−252,659	280.597	−94,878
2,800	55.115	115,472	−252,785	282.595	−89,031
2,900	55.459	121,001	−252,909	284.535	−83,181
3,000	55.779	126,563	−253,034	286.420	−77,326
3,100	56.076	132,156	−253,161	288.254	−71,467
3,200	56.353	137,777	−253,290	290.039	−65,604
3,300	56.610	143,426	−253,423	291.777	−59,737
3,400	56.851	149,099	−253,561	293.471	−53,865
3,500	57.076	154,795	−253,704	295.122	−47,990
3,600	57.288	160,514	−253,852	296.733	−42,110
3,700	57.488	166,252	−254,007	298.305	−36,226
3,800	57.676	172,011	−254,169	299.841	−30,338
3,900	57.856	177,787	−254,338	301.341	−24,446
4,000	58.026	183,582	−254,515	302.808	−18,549
4,100	58.190	189,392	−254,699	304.243	−12,648
4,200	58.346	195,219	−254,892	305.647	−6,742
4,300	58.496	201,061	−255,093	307.022	−831
4,400	58.641	206,918	−255,303	308.368	5,085
4,500	58.781	212,790	−255,522	309.688	11,005
4,600	58.916	218,674	−255,751	310.981	16,930
4,700	59.047	224,573	−255,990	312.250	22,861

Table A.6 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
4,800	59.173	230,484	−256,239	313.494	28,796
4,900	59.295	236,407	−256,501	314.716	34,737
5,000	59.412	242,343	−256,774	315.915	40,684

Table A.7 Nitrogen (N_2), MW = 28.013, enthalpy of formation @ 298 K (kJ/kmol) = 0

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	28.793	−2,841	0	179.959	0
298	29.071	0	0	191.511	0
300	29.075	54	0	191.691	0
400	29.319	2,973	0	200.088	0
500	29.636	5,920	0	206.662	0
600	30.086	8,905	0	212.103	0
700	30.684	11,942	0	216.784	0
800	31.394	15,046	0	220.927	0
900	32.131	18,222	0	224.667	0
1,000	32.762	21,468	0	228.087	0
1,100	33.258	24,770	0	231.233	0
1,200	33.707	28,118	0	234.146	0
1,300	34.113	31,510	0	236.861	0
1,400	34.477	34,939	0	239.402	0
1,500	34.805	38,404	0	241.792	0
1,600	35.099	41,899	0	244.048	0
1,700	35.361	45,423	0	246.184	0
1,800	35.595	48,971	0	248.212	0
1,900	35.803	52,541	0	250.142	0
2,000	35.988	56,130	0	251.983	0
2,100	36.152	59,738	0	253.743	0
2,200	36.298	63,360	0	255.429	0
2,300	36.428	66,997	0	257.045	0
2,400	36.543	70,645	0	258.598	0
2,500	36.645	74,305	0	260.092	0
2,600	36.737	77,974	0	261.531	0
2,700	36.820	81,652	0	262.919	0
2,800	36.895	85,338	0	264.259	0
2,900	36.964	89,031	0	265.555	0
3,000	37.028	92,730	0	266.810	0
3,100	37.088	96,436	0	268.025	0
3,200	37.144	100,148	0	269.203	0
3,300	37.198	103,865	0	270.347	0
3,400	37.251	107,587	0	271.458	0
3,500	37.302	111,315	0	272.539	0
3,600	37.352	115,048	0	273.590	0
3,700	37.402	118,786	0	274.614	0
3,800	37.452	122,528	0	275.612	0
3,900	37.501	126,276	0	276.586	0
4,000	37.549	130,028	0	277.536	0
4,100	37.597	133,786	0	278.464	0
4,200	37.643	137,548	0	279.370	0
4,300	37.688	141,314	0	280.257	0
4,400	37.730	145,085	0	281.123	0
4,500	37.768	148,860	0	281.972	0
4,600	37.803	152,639	0	282.802	0
4,700	37.832	156,420	0	283.616	0

Table A.7 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	37.854	160,205	0	284.412	0
4,900	37.868	163,991	0	285.193	0
5,000	37.873	167,778	0	285.958	0

Table A.8 Nitrogen atom (N), $MW = 14.007$, enthalpy of formation @ 298 K (kJ/kmol) = 472,629

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	20.790	−2,040	472,008	144.889	461,026
298	20.786	0	472,629	153.189	455,504
300	20.786	38	472,640	153.317	455,398
400	20.786	2,117	473,258	159.297	449,557
500	20.786	4,196	473,864	163.935	443,562
600	20.786	6,274	474,450	167.725	437,446
700	20.786	8,353	475,010	170.929	431,234
800	20.786	10,431	475,537	173.705	424,944
900	20.786	12,510	476,027	176.153	418,590
1,000	20.786	14,589	476,483	178.343	412,183
1,100	20.792	16,668	476,911	180.325	405,732
1,200	20.795	18,747	477,316	182.134	399,243
1,300	20.795	20,826	477,700	183.798	392,721
1,400	20.793	22,906	478,064	185.339	386,171
1,500	20.790	24,985	478,411	186.774	379,595
1,600	20.786	27,064	478,742	188.115	372,996
1,700	20.782	29,142	479,059	189.375	366,377
1,800	20.779	31,220	479,363	190.563	359,740
1,900	20.777	33,298	479,656	191.687	353,086
2,000	20.776	35,376	479,939	192.752	346,417
2,100	20.778	37,453	480,213	193.766	339,735
2,200	20.783	39,531	480,479	194.733	333,039
2,300	20.791	41,610	480,740	195.657	326,331
2,400	20.802	43,690	480,995	196.542	319,612
2,500	20.818	45,771	481,246	197.391	312,883
2,600	20.838	47,853	481,494	198.208	306,143
2,700	20.864	49,938	481,740	198.995	299,394
2,800	20.895	52,026	481,985	199.754	292,636
2,900	20.931	54,118	482,230	200.488	285,870
3,000	20.974	56,213	482,476	201.199	279,094
3,100	21.024	58,313	482,723	201.887	272,311
3,200	21.080	60,418	482,972	202.555	265,519
3,300	21.143	62,529	483,224	203.205	258,720
3,400	21.214	64,647	483,481	203.837	251,913
3,500	21.292	66,772	483,742	204.453	245,099
3,600	21.378	68,905	484,009	205.054	238,276
3,700	21.472	71,048	484,283	205.641	231,447
3,800	21.575	73,200	484,564	206.215	224,610
3,900	21.686	75,363	484,853	206.777	217,765
4,000	21.805	77,537	485,151	207.328	210,913
4,100	21.934	79,724	485,459	207.868	204,053
4,200	22.071	81,924	485,779	208.398	197,186
4,300	22.217	84,139	486,110	208.919	190,310
4,400	22.372	86,368	486,453	209.431	183,427
4,500	22.536	88,613	486,811	209.936	176,536
4,600	22.709	90,875	487,184	210.433	169,637
4,700	22.891	93,155	487,573	210.923	162,730

Table A.8 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
4,800	23.082	95,454	487,979	211.407	155,814
4,900	23.282	97,772	488,405	211.885	148,890
5,000	23.491	100,111	488,850	212.358	141,956

Table A.9 Nitric oxide (NO), MW = 30.006, enthalpy of formation @ 298 K (kJ/kmol) = 90,297

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	29.374	−2,901	90,234	198.856	87,811
298	29.728	0	90,297	210.652	86,607
300	29.735	55	90,298	210.836	86,584
400	30.103	3,046	90,341	219.439	85,340
500	30.570	6,079	90,367	226.204	84,086
600	31.174	9,165	90,382	231.829	82,828
700	31.908	12,318	90,393	236.688	81,568
800	32.715	15,549	90,405	241.001	80,307
900	33.489	18,860	90,421	244.900	79,043
1,000	34.076	22,241	90,443	248.462	77,778
1,100	34.483	25,669	90,465	251.729	76,510
1,200	34.850	29,136	90,486	254.745	75,241
1,300	35.180	32,638	90,505	257.548	73,970
1,400	35.474	36,171	90,520	260.166	72,697
1,500	35.737	39,732	90,532	262.623	71,423
1,600	35.972	43,317	90,538	264.937	70,149
1,700	36.180	46,925	90,539	267.124	68,875
1,800	36.364	50,552	90,534	269.197	67,601
1,900	36.527	54,197	90,523	271.168	66,327
2,000	36.671	57,857	90,505	273.045	65,054
2,100	36.797	61,531	90,479	274.838	63,782
2,200	36.909	65,216	90,447	276.552	62,511
2,300	37.008	68,912	90,406	278.195	61,243
2,400	37.095	72,617	90,358	279.772	59,976
2,500	37.173	76,331	90,303	281.288	58,711
2,600	37.242	80,052	90,239	282.747	57,448
2,700	37.305	83,779	90,168	284.154	56,188
2,800	37.362	87,513	90,089	285.512	54,931
2,900	37.415	91,251	90,003	286.824	53,677
3,000	37.464	94,995	89,909	288.093	52,426
3,100	37.511	98,744	89,809	289.322	51,178
3,200	37.556	102,498	89,701	290.514	49,934
3,300	37.600	106,255	89,586	291.670	48,693
3,400	37.643	110,018	89,465	292.793	47,456
3,500	37.686	113,784	89,337	293.885	46,222
3,600	37.729	117,555	89,203	294.947	44,992
3,700	37.771	121,330	89,063	295.981	43,766
3,800	37.815	125,109	88,918	296.989	42,543
3,900	37.858	128,893	88,767	297.972	41,325
4,000	37.900	132,680	88,611	298.931	40,110
4,100	37.943	136,473	88,449	299.867	38,900
4,200	37.984	140,269	88,283	300.782	37,693
4,300	38.023	144,069	88,112	301.677	36,491
4,400	38.060	147,873	87,936	302.551	35,292
4,500	38.093	151,681	87,755	303.407	34,098
4,600	38.122	155,492	87,569	304.244	32,908
4,700	38.146	159,305	87,379	305.064	31,721

Table A.9 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	38.162	163,121	87,184	305.868	30,539
4,900	38.171	166,938	86,984	306.655	29,361
5,000	38.170	170,755	86,779	307.426	28,187

Table A.10 Nitrogen dioxide (NO_2), MW = 46.006, enthalpy of formation @ 298 K (kJ/kmol) = 33, 098

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	32.936	−3,432	33,961	226.016	45,453
298	36.881	0	33,098	239.925	51,291
300	36.949	68	33,085	240.153	51,403
400	40.331	3,937	32,521	251.259	57,602
500	43.227	8,118	32,173	260.578	63,916
600	45.737	12,569	31,974	268.686	70,285
700	47.913	17,255	31,885	275.904	76,679
800	49.762	22,141	31,880	282.427	83,079
900	51.243	27,195	31,938	288.377	89,476
1,000	52.271	32,375	32,035	293.834	95,864
1,100	52.989	37,638	32,146	298.850	102,242
1,200	53.625	42,970	32,267	303.489	108,609
1,300	54.186	48,361	32,392	307.804	114,966
1,400	54.679	53,805	32,519	311.838	121,313
1,500	55.109	59,295	32,643	315.625	127,651
1,600	55.483	64,825	32,762	319.194	133,981
1,700	55.805	70,390	32,873	322.568	140,303
1,800	56.082	75,984	32,973	325.765	146,620
1,900	56.318	81,605	33,061	328.804	152,931
2,000	56.517	87,247	33,134	331.698	159,238
2,100	56.685	92,907	33,192	334.460	165,542
2,200	56.826	98,583	32,233	337.100	171,843
2,300	56.943	104,271	33,256	339.629	178,143
2,400	57.040	109,971	33,262	342.054	184,442
2,500	57.121	115,679	33,248	344.384	190,742
2,600	57.188	121,394	33,216	346.626	197,042
2,700	57.244	127,116	33,165	348.785	203,344
2,800	57.291	132,843	33,095	350.868	209,648
2,900	57.333	138,574	33,007	352.879	215,955
3,000	57.371	144,309	32,900	354.824	222,265
3,100	57.406	150,048	32,776	356.705	228,579
3,200	57.440	155,791	32,634	358.529	234,898
3,300	57.474	161,536	32,476	360.297	241,221
3,400	57.509	167,285	32,302	362.013	247,549
3,500	57.546	173,038	32,113	363.680	253,883
3,600	57.584	178,795	31,908	365.302	260,222
3,700	57.624	184,555	31,689	366.880	266,567
3,800	57.665	190,319	31,456	368.418	272,918
3,900	57.708	196,088	31,210	369.916	279,276
4,000	57.750	201,861	30,951	371.378	285,639
4,100	57.792	207,638	30,678	372.804	292,010
4,200	57.831	213,419	30,393	374.197	298,387
4,300	57.866	219,204	30,095	375.559	304,772
4,400	57.895	224,992	29,783	376.889	311,163
4,500	57.915	230,783	29,457	378.190	317,562
4,600	57.925	236,575	29,117	379.464	323,968
4,700	57.922	242,367	28,761	380.709	330,381

Table A.10 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	57.902	248,159	28,389	381.929	336,803
4,900	57.862	253,947	27,998	383.122	343,232
5,000	57.798	259,730	27,586	384.290	349,670

Table A.11 Oxygen (O_2), MW = 31.999, enthalpy of formation @ 298 K (kJ/kmol) = 0

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	28.473	−2,836	0	193.518	0
298	29.315	0	0	205.043	0
300	29.331	54	0	205.224	0
400	30.210	3,031	0	213.782	0
500	31.114	6,097	0	220.620	0
600	32.030	9,254	0	226.374	0
700	32.927	12,503	0	231.379	0
800	33.757	15,838	0	235.831	0
900	34.454	19,250	0	239.849	0
1,000	34.936	22,721	0	243.507	0
1,100	35.270	26,232	0	246.852	0
1,200	35.593	29,775	0	249.935	0
1,300	35.903	33,350	0	252.796	0
1,400	36.202	36,955	0	255.468	0
1,500	36.490	40,590	0	257.976	0
1,600	36.768	44,253	0	260.339	0
1,700	37.036	47,943	0	262.577	0
1,800	37.296	51,660	0	264.701	0
1,900	37.546	55,402	0	266.724	0
2,000	37.788	59,169	0	268.656	0
2,100	38.023	62,959	0	270.506	0
2,200	38.250	66,773	0	272.280	0
2,300	38.470	70,609	0	273.985	0
2,400	38.684	74,467	0	275.627	0
2,500	38.891	78,346	0	277.210	0
2,600	39.093	82,245	0	278.739	0
2,700	39.289	86,164	0	280.218	0
2,800	39.480	90,103	0	281.651	0
2,900	39.665	94,060	0	283.039	0
3,000	39.846	98,036	0	284.387	0
3,100	40.023	102,029	0	285.697	0
3,200	40.195	106,040	0	286.970	0
3,300	40.362	110,068	0	288.209	0
3,400	40.526	114,112	0	289.417	0
3,500	40.686	118,173	0	290.594	0
3,600	40.842	122,249	0	291.742	0
3,700	40.994	126,341	0	292.863	0
3,800	41.143	130,448	0	293.959	0
3,900	41.287	134,570	0	295.029	0
4,000	41.429	138,705	0	296.076	0
4,100	41.566	142,855	0	297.101	0
4,200	41.700	147,019	0	298.104	0
4,300	41.830	151,195	0	299.087	0
4,400	41.957	155,384	0	300.050	0
4,500	42.079	159,586	0	300.994	0
4,600	42.197	163,800	0	301.921	0
4,700	42.312	168,026	0	302.829	0

Table A.11 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	42.421	172,262	0	303.721	0
4,900	42.527	176,510	0	304.597	0
5,000	42.627	180,767	0	305.457	0

Table A.12 Oxygen atom (O), MW = 16.000, enthalpy of formation @ 298 K (kJ/kmol) = 249,197

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
200	22.477	−2,176	248,439	152.085	237,374
298	21.899	0	249,197	160.945	231,778
300	21.890	41	249,211	161.080	231,670
400	21.500	2,209	249,890	167.320	225,719
500	21.256	4,345	250,494	172.089	219,605
600	21.113	6,463	251,033	175.951	213,375
700	21.033	8,570	251,516	179.199	207,060
800	20.986	10,671	251,949	182.004	200,679
900	20.952	12,768	252,340	184.474	194,246
1,000	20.915	14,861	252,698	186.679	187,772
1,100	20.898	16,952	253,033	188.672	181,263
1,200	20.882	19,041	253,350	190.490	174,724
1,300	20.867	21,128	253,650	192.160	168,159
1,400	20.854	23,214	253,934	193.706	161,572
1,500	20.843	25,299	254,201	195.145	154,966
1,600	20.834	27,383	254,454	196.490	148,342
1,700	20.827	29,466	254,692	197.753	141,702
1,800	20.822	31,548	254,916	198.943	135,049
1,900	20.820	33,630	255,127	200.069	128,384
2,000	20.819	35,712	255,325	201.136	121,709
2,100	20.821	37,794	255,512	202.152	115,023
2,200	20.825	39,877	255,687	203.121	108,329
2,300	20.831	41,959	255,852	204.047	101,627
2,400	20.840	44,043	256,007	204.933	94,918
2,500	20.851	46,127	256,152	205.784	88,203
2,600	20.865	48,213	256,288	206.602	81,483
2,700	20.881	50,300	256,416	207.390	74,757
2,800	20.899	52,389	256,535	208.150	68,027
2,900	20.920	54,480	256,648	208.884	61,292
3,000	20.944	56,574	256,753	209.593	54,554
3,100	20.970	58,669	256,852	210.280	47,812
3,200	20.998	60,768	256,945	210.947	41,068
3,300	21.028	62,869	257,032	211.593	34,320
3,400	21.061	64,973	257,114	212.221	27,570
3,500	21.095	67,081	257,192	212.832	20,818
3,600	21.132	69,192	257,265	213.427	14,063
3,700	21.171	71,308	257,334	214.007	7,307
3,800	21.212	73,427	257,400	214.572	548
3,900	21.254	75,550	257,462	215.123	−6,212
4,000	21.299	77,678	257,522	215.662	−12,974
4,100	21.345	79,810	257,579	216.189	−19,737
4,200	21.392	81,947	257,635	216.703	−26,501
4,300	21.441	84,088	257,688	217.207	−33,267
4,400	21.490	86,235	257,740	217.701	−40,034
4,500	21.541	88,386	257,790	218.184	−46,802
4,600	21.593	90,543	257,840	218.658	−53,571
4,700	21.646	92,705	257,889	219.123	−60,342

Table A.12 (continued)

T(K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}^o_f(298))$ (kJ/kmol)	$\bar{h}^o_f(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}^o_f(T)$ (kJ/kmol)
4,800	21.699	94,872	257,938	219.580	−67,113
4,900	21.752	97,045	257,987	220.028	−73,886
5,000	21.805	99,223	258,036	220.468	−80,659

Table A.13 Curvefit coefficients for thermodynamic properties (C–H–O–N system)

$$\bar{c}_p/R_u = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\bar{h}^\circ/R_uT = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T}$$

$$\bar{s}^\circ/R_u = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7$$

Species	T(K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
CO	1,000–5,000	0.03025078E+02	0.14426885E−02	−0.05630827E−05	0.10185813E−09	−0.06910951E−13	−0.14268350E+05	0.06108217E+02
	300–1,000	0.03262451E+02	0.15119409E−02	−0.03881755E−04	0.05581944E−07	−0.02474951E−10	−0.14310539E+05	0.04848897E+02
CO_2	1,000–5,000	0.04453623E+02	0.03140168E−01	−0.12784105E−05	0.02393996E−08	−0.16690333E−13	−0.04896696E+06	−0.09553959E+01
	300–1,000	0.02275724E+02	0.09922072E−01	−0.10409113E−04	0.06866686E−07	−0.02117280E−10	−0.04837314E+06	0.10188488E+02
H_2	1,000–5,000	0.02991423E+02	0.07000644E−02	−0.05633828E−06	−0.09231578E−10	0.15827519E−14	−0.08350340E+04	−0.13551101E+01
	300–1,000	0.03298124E+02	0.08249441E−02	−0.08143015E−05	−0.09475434E−09	0.04134872E−11	−0.10125209E+04	−0.03294094E+02
H	1,000–5,000	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	−0.04601176E+01
	300–1,000	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	−0.04601176E+01
OH	1,000–5,000	0.02882730E+02	0.10139743E−02	−0.02276877E−05	0.02174683E−09	−0.05126305E−14	0.03886888E+05	0.05595712E+02
	300–1,000	0.03637266E+02	0.01850910E−02	−0.16761646E−05	0.02387202E−07	−0.08431442E−11	0.03606781E+05	0.13588605E+01
H_2O	1,000–5,000	0.02672145E+02	0.03056293E−01	−0.08730260E−05	0.12009964E−09	−0.06391618E−13	−0.02989921E+06	0.06862817E+02
	300–1,000	0.03386842E+02	0.03474982E−01	−0.06354696E−04	0.06968581E−07	−0.02506588E−10	−0.03020811E+06	0.02590232E+02
N_2	1,000–5,000	0.02926640E+02	0.14879768E−02	−0.05684760E−05	0.10097038E−09	−0.06753351E−13	−0.09227977E+04	0.05980528E+02
	300–1,000	0.03298677E+02	0.14082404E−02	−0.03963222E−04	0.05641515E−07	−0.02444854E−10	−0.10208999E+04	0.03950372E+02
N	1,000–5,000	0.02450268E+02	0.10661458E−03	−0.07465337E−06	0.01879652E−09	−0.10259839E−14	0.05611604E+06	0.04448758E+02
	300–1,000	0.02503071E+02	−0.02180018E−03	0.05420529E−06	−0.05647560E−09	0.02099904E−12	0.05609890E+06	0.04167566E+02
NO	1,000–5,000	0.03245435E+02	0.12691383E−02	−0.05015890E−05	0.09169283E−09	−0.06275419E−13	0.09800840E+05	0.06417293E+02
	300–1,000	0.03376541E+02	0.12530634E−02	−0.03302750E−04	0.05217810E−07	−0.02446262E−10	0.09817961E+05	0.05829590E+02
NO_2	1,000–5,000	0.04682859E+02	0.02462429E−01	−0.10422585E−05	0.01976902E−08	−0.13917168E−13	0.02261292E+05	0.09885985E+01
	300–1,000	0.02670600E+02	0.07838500E−01	−0.08063864E−04	0.06161714E−07	−0.02320150E−10	0.02896290E+05	0.11612071E+02

Table A.13 (continued)

Species	T(K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
O_2	1,000-5,000	0.03697578E+02	0.06135197E−02	−0.12588420E−06	0.01775281E−09	−0.11364354E−14	−0.12339301E+04	0.03189165E+02
	300–1,000	0.03212936E+02	0.11274864E−02	−0.05756150E−05	0.13138773E−08	−0.08768554E−11	−0.10052490E+04	0.06034737E+02
O	1,000–5,000	0.02542059E+02	−0.02755061E−03	−0.03102803E−07	0.04551067E−10	−0.04368051E−14	0.02923080E+06	0.04920308E+02
	300–1,000	0.02946428E+02	−0.16381665E−02	0.02421031E−04	−0.16028431E−08	0.03890696E−11	0.02914764E+06	0.02963995E+02

SOURCE: Kee, R. J., Rupley, F. M., and Miller, J. A., "The Chemkin Thermodynamic Data Base," Sandia Report, SAND87-8215B, reprinted March 1991.

APPENDIX

B

FUEL PROPERTIES

Table B.1 Selected properties of hydrocarbon fuels: enthalpy of formation,[a] Gibbs function of formation,[a] entropy,[a] and higher and lower heating values all at 298.15 K and 1 atm; boiling points[b] and latent heat of vaporization[c] at 1 atm; constant-pressure adiabatic flame temperature at 1 atm;[d] liquid density[c]

Formula	Fuel	MW (kg/kmol)	$\bar{h}_f^o$ (kJ/kmol)	$\bar{g}_f^o$ (kJ/kmol)	$\bar{s}^o$ (kJ/kmol-K)	HHV† (kJ/kg)	LHV† (kJ/kg)	Boiling pt. (°C)	h_{fg} (kJ/kg)	$T_{ad}^{\ddagger}$ (K)	ρ_{liq}^* (kg/m³)
CH_4	Methane	16.043	−74,831	−50,794	186.188	55,528	50,016	−164	509	2,226	300
C_2H_2	Acetylene	26.038	226,748	209,200	200.819	49,923	48,225	−84	—	2,539	—
C_2H_4	Ethene	28.054	52,283	68,124	219.827	50,313	47,161	−103.7	—	2,369	—
C_2H_6	Ethane	30.069	−84,667	−32,886	229.492	51,901	47,489	−88.6	488	2,259	370
C_3H_6	Propene	42.080	20,414	62,718	266.939	48,936	45,784	−47.4	437	2,334	514
C_3H_8	Propane	44.096	−103,847	−23,489	269.910	50,368	46,357	−42.1	425	2,267	500
C_4H_8	1-Butene	56.107	1,172	72,036	307.440	48,471	45,319	−63	391	2,322	595
C_4H_{10}	*n*-Butane	58.123	−124,733	−15,707	310.034	49,546	45,742	−0.5	386	2,270	579
C_5H_{10}	1-Pentene	70.134	−20,920	78,605	347.607	48,152	45,000	30	358	2,314	641
C_5H_{12}	*n*-Pentane	72.150	−146,440	−8,201	348.402	49,032	45,355	36.1	358	2,272	626
C_6H_6	Benzene	78.113	82,927	129,658	269.199	42,277	40,579	80.1	393	2,342	879
C_6H_{12}	1-Hexene	84.161	−41,673	87,027	385.974	47,955	44,803	63.4	335	2,308	673
C_6H_{14}	*n*-Hexane	86.177	−167,193	209	386.811	48,696	45,105	69	335	2,273	659
C_7H_{14}	1-Heptene	98.188	−62,132	95,563	424.383	47,817	44,665	93.6	—	2,305	—
C_7H_{16}	*n*-Heptane	100.203	−187,820	8,745	425.262	48,456	44,926	98.4	316	2,274	684
C_8H_{16}	1-Octene	112.214	−82,927	104,140	462.792	47,712	44,560	121.3	—	2,302	—
C_8H_{18}	*n*-Octane	114.230	−208,447	17,322	463.671	48,275	44,791	125.7	300	2,275	703
C_9H_{18}	1-Nonene	126.241	−103,512	112,717	501.243	47,631	44,478	—	—	2,300	—
C_9H_{20}	*n*-Nonane	128.257	−229,032	25,857	502.080	48,134	44,686	150.8	295	2,276	718
$C_{10}H_{20}$	1-Decene	140.268	−124,139	121,294	539.652	47,565	44,413	170.6	—	2,298	—
$C_{10}H_{22}$	*n*-Decane	142.284	−249,659	34,434	540.531	48,020	44,602	174.1	277	2,277	730
$C_{11}H_{22}$	1-Undecene	154.295	−144,766	129,830	578.061	47,512	44,360	—	—	2,296	—
$C_{11}H_{24}$	*n*-Undecane	156.311	−270,286	43,012	578.940	47,926	44,532	195.9	265	2,277	740

Table B.1 (continued)

Formula	Fuel	*MW* (kg/kmol)	$\bar{h}_f^o$ (kJ/kmol)	$\bar{g}_f^o$ (kJ/kmol)	$\bar{s}^o$ (kJ/kmol-K)	HHV† (kJ/kg)	LHV† (kJ/kg)	Boiling pt. (°C)	h_{fg} (kJ/kg)	$T_{ad}^{‡}$ (K)	ρ_{liq}^{*} (kg/m^3)
$C_{12}H_{24}$	1-Dodecene	168.322	−165,352	138,407	616.471	47,468	44,316	213.4	—	2,295	—
$C_{12}H_{26}$	*n*-Dodecane	170.337	−292,162	—	—	47,841	44,467	216.3	256	2,277	749

† Based on gaseous fuel.

‡ For stoichiometric combustion with air (79 percent N_2, 21 percent O_2).

* For liquids at 20°C or for gases at the boiling point of the liquefied gas.

SOURCES:

[a] Rossini, F. D., *et al.*, *Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds*, Carnegie Press, Pittsburgh, PA, 1953.

[b] Weast, R. C. (ed.), *Handbook of Chemistry and Physics*, 56th Ed., CRC Press, Cleveland, OH, 1976.

[c] Obert, E. F., *Internal Combustion Engines and Air Pollution*, Harper & Row, New York, 1973.

[d] Calculated using HPFLAME (Appendix F).

Table B.2 Curvefit coefficients for fuel specific heat and enthalpy[a] for reference state of zero enthalpy of the elements at 298.15 K, 1 atm

$$\bar{c}_p\ (\text{kJ/kmol-K}) = 4.184(a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2}),$$

$$\bar{h}^o\ (\text{kJ/kmol}) = 4184\,(a_1\theta + a_2\theta^2/2 + a_3\theta^3/3 + a_4\theta^4/4 - a_5\theta^{-1} + a_6),$$

$$\text{where } \theta \equiv T\,(\text{K})/1000$$

Formula	Fuel	*MW*	a_1	a_2	a_3	a_4	a_5	a_6	a_8[b]
CH_4	Methane	16.043	−0.29149	26.327	−10.610	1.5656	0.16573	−18.331	4.300
C_3H_8	Propane	44.096	−1.4867	74.339	−39.065	8.0543	0.01219	−27.313	8.852
C_6H_{14}	Hexane	86.177	−20.777	210.48	−164.125	52.832	0.56635	−39.836	15.611
C_8H_{18}	Isooctane	114.230	−0.55313	181.62	−97.787	20.402	−0.03095	−60.751	20.232
CH_3OH	Methanol	32.040	−2.7059	44.168	−27.501	7.2193	0.20299	−48.288	5.3375
C_2H_5OH	Ethanol	46.07	6.990	39.741	−11.926	0	0	−60.214	7.6135
$C_{8.26}H_{15.5}$	Gasoline	114.8	−24.078	256.63	−201.68	64.750	0.5808	−27.562	17.792
$C_{7.76}H_{13.1}$		106.4	−22.501	227.99	−177.26	56.048	0.4845	−17.578	15.232
$C_{10.8}H_{18.7}$	Diesel	148.6	−9.1063	246.97	−143.74	32.329	0.0518	−50.128	23.514

[a] SOURCE: From Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, by permission of McGraw-Hill, Inc.

[b] To obtain 0 K reference state for enthalpy, add a_8 to a_6.

Table B.3 Curvefit coefficients for fuel vapor thermal conductivity, viscosity, and specific heat[a]

$$\left.\begin{array}{l} k\,(\mathrm{W/m\text{-}K}) \\ \mu\,(\mathrm{N\text{-}s/m^2})\cdot 10^6 \\ c_p\,(\mathrm{J/kg\text{-}K}) \end{array}\right\} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 + a_6T^5 + a_7T^6$$

Formula	Fuel	T-range (K)	Property	a_1	a_2	a_3	a_4	a_5	a_6	a_7
CH_4	Methane	100–1,000	k	−1.34014990E−2	3.66307060E−4	−1.82248608E−6	5.93987998E−9	−9.14055050E−12	−6.78968890E−15	−1.95048736E−18
		70–1,000	μ	2.96826700E−1	3.71120100E−2	1.21829800E−5	−7.02426000E−8	7.54326900E−11	−2.72371660E−14	0
			c_p	See Table B.2						
C_3H_8	Propane	200–500	k	−1.07682209E−2	8.38590325E−5	4.22059864E−8	0	0	0	0
		270–600	μ	−3.54371100E−1	3.08009600E−2	−6.99723000E−6	0	0	0	0
			c_p	See Table B.2						
C_6H_{14}	*n*-Hexane	150–1,000	k	1.28775700E−3	−2.00499443E−5	2.37858831E−7	−1.60944555E−10	7.71027290E−14	0	0
		270–900	μ	1.54541200E+0	1.15080900E−2	2.72216500E−5	−3.26900000E− 8	1.24545900E−11	0	0
			c_p	See Table B.2						
C_7H_{16}	*n*-Heptane	250–1,000	k	−4.60614700E−2	5.95652224E−4	−2.98893153E−6	8.44612876E−9	−1.22927E−11	9.0127E−15	−2.62961E−18
		270–580	μ	1.54009700E+0	1.09515700E−2	1.80066400E−5	−1.36379000E−8	0	0	0
		300–755	c_p	9.46260000E+1	5.86099700E+0	−1.98231320E−3	−6.88699300E−8	−1.93795260E−10	0	0
		755–1,365	c_p	−7.40308000E+2	1.08935370E+1	−1.26512400E−2	9.84376300E−6	−4.32282960E−9	7.86366500E−13	0
C_8H_{18}	*n*-Octane	250–500	k	−4.01391940E−3	3.38796092E−5	8.19291819E−8	0	0	0	0
		300–650	μ	8.32435400E−1	1.40045000E−2	8.79376500E−6	−6.84030000E−9	0	0	0
		275–755	c_p	2.14419800E+2	5.35690500E+0	−1.17497000E−3	−6.99115500E−7	0	0	0
		755–1,365	c_p	2.43596860E+3	−4.46819470E+0	−1.66843290E−2	−1.78856050E−5	8.64282020E−9	−1.61426500E−12	0
$C_{10}H_{22}$	*n*-Decane	250–500	k	−5.88274000E−3	3.72449646E−5	7.55109624E−8	0	0	0	0
			μ	Not available						
		300-700	c_p	2.40717800E+2	5.09965000E+0	−6.29026000E−4	−1.07155000E−6	0	0	0
		700–1,365	c_p	−1.35345890E+4	9.14879000E+1	−2.20700000E−1	2.91406000E−4	−2.15307400E−7	8.38600000E−11	−1.34404000E−14
CH_3OH	Methanol	300–550	k	−2.02986750E−2	1.21910927E−4	−2.23748473E−8	0	0	0	0
		250–650	μ	1.19790000E+0	2.45028000E−2	1.86162740E−5	−1.30674820E−8	0	0	0
			c_p	See Table B.2						
C_2H_5OH	Ethanol	250–550	k	−2.46663000E−2	1.55892550E−4	−8.22954822E−8	0	0	0	0
		270–600	μ	−6.33595000E−2	3.20713470E−2	−6.25079576E−6	0	0	0	0
			c_p	See Table B.2						

[a] SOURCE: Andrews, J. R., and Biblarz, O., "Temperature Dependence of Gas Properties in Polynomial Form," Naval Postgraduate School, NPS67-81-001, January 1981.

APPENDIX

C

SELECTED PROPERTIES OF AIR, NITROGEN, AND OXYGEN

Table C.1 Selected properties of air at 1 atm[a]

T (K)	ρ (kg/m^3)	c_p (kJ/kg-K)	$\mu \cdot 10^7$ (N-s/m^2)	$\nu \cdot 10^6$ (m^2/s)	$k \cdot 10^3$ (W/m-K)	$\alpha \cdot 10^6$ (m^2/s)	Pr
100	3.5562	1.032	71.1	2.00	9.34	2.54	0.786
150	2.3364	1.012	103.4	4.426	13.8	5.84	0.758
200	1.7458	1.007	132.5	7.590	18.1	10.3	0.737
250	1.3947	1.006	159.6	11.44	22.3	15.9	0.720
300	1.1614	1.007	184.6	15.89	26.3	22.5	0.707
350	0.9950	1.009	208.2	20.92	30.0	29.9	0.700
400	0.8711	1.014	230.1	26.41	33.8	38.3	0.690
450	0.7740	1.021	250.7	32.39	37.3	47.2	0.686
500	0.6964	1.030	270.1	38.79	40.7	56.7	0.684
550	0.6329	1.040	288.4	45.57	43.9	66.7	0.683
600	0.5804	1.051	305.8	52.69	46.9	76.9	0.685
650	0.5356	1.063	322.5	60.21	49.7	87.3	0.690
700	0.4975	1.075	338.8	68.10	52.4	98.0	0.695
750	0.4643	1.087	354.6	76.37	54.9	109	0.702
800	0.4354	1.099	369.8	84.93	57.3	120	0.709
850	0.4097	1.110	384.3	93.80	59.6	131	0.716
900	0.3868	1.121	398.1	102.9	62.0	143	0.720
950	0.3666	1.131	411.3	112.2	64.3	155	0.723
1,000	0.3482	1.141	424.4	121.9	66.7	168	0.726
1,100	0.3166	1.159	449.0	141.8	71.5	195	0.728
1,200	0.2902	1.175	473.0	162.9	76.3	224	0.728
1,300	0.2679	1.189	496.0	185.1	82	238	0.719
1,400	0.2488	1.207	530	213	91	303	0.703
1,500	0.2322	1.230	557	240	100	350	0.685
1,600	0.2177	1.248	584	268	106	390	0.688

Table C.1 (continued)

T (K)	ρ (kg/m^3)	c_p (kJ/kg-K)	$\mu \cdot 10^7$ (N-s/m^2)	$\nu \cdot 10^6$ (m^2/s)	$k \cdot 10^3$ (W/m-K)	$\alpha \cdot 10^6$ (m^2/s)	Pr
1,700	0.2049	1.267	611	298	113	435	0.685
1,800	0.1935	1.286	637	329	120	482	0.683
1,900	0.1833	1.307	663	362	128	534	0.677
2,000	0.1741	1.337	689	396	137	589	0.672
2,100	0.1658	1.372	715	431	147	646	0.667
2,200	0.1582	1.417	740	468	160	714	0.655
2,300	0.1513	1.478	766	506	175	783	0.647
2,400	0.1448	1.558	792	547	196	869	0.630
2,500	0.1389	1.665	818	589	222	960	0.613
3,000	0.1135	2.726	955	841	486	1,570	0.536

[a] SOURCE: Incropera, F. P., and DeWitt, D. P., *Fundamentals of Heat and Mass Transfer*, 3rd Ed. Reprinted by permission, ©1990, John Wiley & Sons, Inc.

Table C.2 Selected properties of nitrogen and oxygen at 1 atm[a]

T (K)	ρ (kg/m^3)	c_p (kJ/kg-K)	$\mu \cdot 10^7$ (N-s/m^2)	$\nu \cdot 10^6$ (m^2/s)	$k \cdot 10^3$ (W/m-K)	$\alpha \cdot 10^6$ (m^2/s)	Pr
Nitrogen (N_2)							
100	3.4388	1.070	68.8	2.00	9.58	2.60	0.768
150	2.2594	1.050	100.6	4.45	13.9	5.86	0.759
200	1.6883	1.043	129.2	7.65	18.3	10.4	0.736
250	1.3488	1.042	154.9	11.48	22.2	15.8	0.727
300	1.1233	1.041	178.2	15.86	25.9	22.1	0.716
350	0.9625	1.042	200.0	20.78	29.3	29.2	0.711
400	0.8425	1.045	220.4	26.16	32.7	37.1	0.704
450	0.7485	1.050	239.6	32.01	35.8	45.6	0.703
500	0.6739	1.056	257.7	38.24	38.9	54.7	0.700
550	0.6124	1.065	274.7	44.86	41.7	63.9	0.702
600	0.5615	1.075	290.8	51.79	44.6	73.9	0.701
700	0.4812	1.098	321.0	66.71	49.9	94.4	0.706
800	0.4211	1.22	349.1	82.90	54.8	116	0.715
900	0.3743	1.146	375.3	100.3	59.7	139	0.721
1,000	0.3368	1.167	399.9	118.7	64.7	165	0.721
1,100	0.3062	1.187	423.2	138.2	70.0	193	0.718
1,200	0.2807	1.204	445.3	158.6	75.8	224	0.707
1,300	0.2591	1.219	466.2	179.9	81.0	256	0.701
Oxygen (O_2)							
100	3.945	0.962	76.4	1.94	9.25	2.44	0.796
150	2.585	0.921	114.8	4.44	13.8	5.80	0.766
200	1.930	0.915	147.5	7.64	18.3	10.4	0.737
250	1.542	0.915	178.6	11.58	22.6	16.0	0.723
300	1.284	0.920	207.2	16.14	26.8	22.7	0.711
350	1.100	0.929	233.5	21.23	29.6	29.0	0.733
400	0.9620	0.942	258.2	26.84	33.0	36.4	0.737
450	0.8554	0.956	281.4	32.90	36.3	44.4	0.741
500	0.7698	0.972	303.3	39.40	41.2	55.1	0.716
550	0.6998	0.988	324.0	46.30	44.1	63.8	0.726
600	0.6414	1.003	343.7	53.59	47.3	73.5	0.729
700	0.5498	1.031	380.8	69.26	52.8	93.1	0.744
800	0.4810	1.054	415.2	86.32	58.9	116	0.743
900	0.4275	1.074	447.2	104.6	64.9	141	0.740
1,000	0.3848	1.090	477.0	124.0	71.0	169	0.733
1,100	0.3498	1.103	505.5	144.5	75.8	196	0.736
1,200	0.3206	1.115	532.5	166.1	81.9	229	0.725
1,300	0.2960	1.125	588.4	188.6	87.1	262	0.721

[a] SOURCE: Incropera, F. P., and DeWitt, D. P., *Fundamentals of Heat and Mass Transfer*, 3rd Ed. Reprinted by permission, © 1990 John Wiley & Sons, Inc.

APPENDIX

D

BINARY DIFFUSION COEFFICIENTS AND METHODOLOGY FOR THEIR ESTIMATION

Table D.1 Binary diffusion coefficients at 1 atm[a,b]

Substance A	Substance B	T (K)	$\mathcal{D}_{AB} \cdot 10^5$ (m^2/s)
Benzene	Air	273	0.77
Carbon dioxide	Air	273	1.38
Carbon dioxide	Nitrogen	293	1.63
Cyclohexane	Air	318	0.86
n-Decane	Nitrogen	363	0.84
n-Dodecane	Nitrogen	399	0.81
Ethanol	Air	273	1.02
n-Hexane	Nitrogen	288	0.757
Hydrogen	Air	273	0.611
Methanol	Air	273	1.32
n-Octane	Air	273	0.505
n-Octane	Nitrogen	303	0.71
Toluene	Air	303	0.88
2,2,4-Trimethyl pentane (Isooctane)	Nitrogen	303	0.705
2,2,3-Trimethyl heptane	Nitrogen	363	0.684
Water	Air	273	2.2

[a] SOURCE: Perry, R. H., Green, D. W., and Maloney, J. O., *Perry's Chemical Engineers' Handbook*, 6th Ed., McGraw-Hill, New York, 1984.

[b] Assuming ideal-gas behavior, the pressure and temperature dependence of the binary diffusion coefficient can be estimated using $\mathcal{D}_{AB} \propto T^{3/2}/P$.

PREDICTING BINARY DIFFUSION COEFFICIENTS FROM THEORY

The following approach for predicting binary diffusion coefficients is a brief summary of that presented by Reid *et al.* [1]. The methodology is based on the Chapman–Enskog theoretical description of binary mixtures of gases at low to moderate pressures. In this theory, the binary diffusion coefficient for the species pair A and B is

$$\mathcal{D}_{\rm AB} = \frac{3}{16}\frac{(4\pi k_B T/MW_{\rm AB})^{1/2}}{(P/R_u T)\pi\sigma_{\rm AB}^2\Omega_D} f_D, \tag{D.1}$$

where k_B is the Boltzmann constant, T (K) is the absolute temperature, P (Pa) is the pressure, R_u is the universal gas constant, and f_D is a theoretical correction factor whose value is sufficiently close to unity to be assumed to be the same. The remaining terms are defined below:

$$MW_{\rm AB} = 2[(1/MW_{\rm A}) + (1/MW_{\rm B})]^{-1}, \tag{D.2}$$

where $MW_{\rm A}$ and $MW_{\rm B}$ are the molecular weights of species A and B, respectively;

$$\sigma_{\rm AB} = (\sigma_{\rm A} + \sigma_{\rm B})/2, \tag{D.3}$$

where $\sigma_{\rm A}$ and $\sigma_{\rm B}$ are the hard-sphere collision diameters of species A and B, respectively, values of which are shown in Table D.2 for several species of interest in combustion.

The collision integral, Ω_D, is a dimensionless quantity calculated using the following expression:

$$\Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}, \tag{D.4}$$

where

$A = 1.06036,\quad B = 0.15610,$
$C = 0.19300,\quad D = 0.47635,$
$E = 1.03587,\quad F = 1.52996,$
$G = 1.76474,\quad H = 3.89411,$

and where the dimensionless temperature T^* is defined by

$$T^* = k_B T/\varepsilon_{\rm AB} = k_B T/(\varepsilon_{\rm A}\varepsilon_{\rm B})^{1/2}. \tag{D.5}$$

Values of the characteristic Lennard–Jones energy, ε_i, are also tabulated in Table D.2 [1].

Table D.2 Lennard–Jones parameters for selected species [2]

Species	σ (Å)	ε/k_B (K)	Species	σ (Å)	ε/k_B (K)
Air	3.711	78.6	n-C_5H_{12}	5.784	341.1
Al	2.655	2750	C_6H_6	5.349	412.3
Ar	3.542	93.3	C_6H_{12}	6.182	297.1
B	2.265	3331	n-C_6H_{14}	5.949	399.3
BO	2.944	596	H	2.708	37.0
B_2O_3	4.158	2092	H_2	2.827	59.7
C	3.385	30.6	H_2O	2.641	809.1
CH	3.370	68.7	H_2O_2	4.196	389.3
CH_3OH	3.626	481.8	He	2.551	10.22
CH_4	3.758	148.6	N	3.298	71.4
CN	3.856	75	NH_3	2.900	558.3
CO	3.690	91.7	NO	3.492	116.7
CO_2	3.941	195.2	N_2	3.798	71.4
C_2H_2	4.033	231.8	N_2O	3.828	232.4
C_2H_4	4.163	224.7	O	3.050	106.7
C_2H_6	4.443	215.7	OH	3.147	79.8
C_3H_8	5.118	237.1	O_2	3.467	106.7
n-C_3H_7OH	4.549	576.7	S	3.839	847
n-C_4H_{10}	4.687	531.4	SO	3.993	301
iso-C_4H_{10}	5.278	330.1	SO_2	4.112	335.4

Substituting numerical values for the constants in Eqn. D.1 results in

$$\mathcal{D}_{AB} = \frac{0.0266 T^{3/2}}{P MW_{AB}^{1/2} \sigma_{AB}^2 \Omega_D} \tag{D.6}$$

with the following associated units: $\mathcal{D}_{AB}[=]\,m^2/s$, $T[=]\,K$, $P[=]\,Pa$, and $\sigma_{AB}[=]\,Å$.

REFERENCES

1. Reid, R. C., Prausnitz, J. M., and Poling, B. E., *The Properties of Gases and Liquids*, 4th Ed., McGraw-Hill, New York, 1987.
2. Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA Technical Report R-132, 1962.

APPENDIX

E

GENERALIZED NEWTON'S METHOD FOR THE SOLUTION OF NONLINEAR EQUATIONS

The Newton–Raphson method, Eqn. E.1, can be extended and applied to a system of nonlinear equations, Eqn. E.2:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{f(x_k)}{\dfrac{\mathrm{d}f}{\mathrm{d}x}(x_k)}; \qquad k \equiv \text{ iteration.} \tag{E.1}$$

System:

$$\begin{aligned} f_1(x_1, x_2, x_3, \ldots, x_n) &= 0, \\ f_2(x_1, x_2, x_3, \ldots, x_n) &= 0, \\ &\vdots \\ f_n(x_1, x_2, x_3, \ldots, x_n) &= 0. \end{aligned} \tag{E.2}$$

Each of these may be expanded in Taylor's series form (truncating second-order and higher terms) as

$$f_i(\tilde{x} + \tilde{\delta}) = f_i(\tilde{x}) + \frac{\partial f_i}{\partial x_1}\delta_1 + \frac{\partial f_i}{\partial x_2}\delta_2 + \frac{\partial f_i}{\partial x_3}\delta_3 + \ldots + \frac{\partial f_i}{\partial x_n}\delta_n, \tag{E.3}$$

for $i = 1, 2, 3, \ldots, n$, where

$$\tilde{x} \equiv \{x\}.$$

At the solution, $f(\tilde{x} + \tilde{\delta}) \rightarrow 0$; the above can be arranged as a set of *linear* equations in the matrix form,

$$\left[\frac{\partial f}{\partial x}\right]\{\delta\} = -\{f\};$$

that is,

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} \begin{Bmatrix} \delta_1 \\ \vdots \\ \delta_n \end{Bmatrix} = \begin{Bmatrix} -f_1 \\ \vdots \\ -f_n \end{Bmatrix} \tag{E.4}$$

where the coefficient matrix on the left-hand-side is called the **Jacobian.**

Equation E.4 may be solved (for δ) using Gauss elimination; once δ is known, the next (better) approximation is found from the recursion relation,

$$\{x\}_{k+1} = \{x\}_k + \{\delta\}_k.$$

The process of forming the Jacobian, solving Eqn. E.4, and calculating new values for $\{x\}$ is repeated until a stop criterion is met. The following is suggested by Suh and Radcliffe [1]:

Stop criterion	*Condition*
$\lvert\delta_j/x_j\rvert \leq 10^{-7}$	$\lvert x_j\rvert \geq 10^{-7}$
or	
$\lvert\delta_j\rvert \leq 10^{-7}$	$\lvert x_j\rvert \leq 10^{-7}$

for $j = 1, 2, 3, \ldots, n$.

Estimates to the partial derivatives may be formed numerically from

$$\frac{\partial f_i}{\partial x_j} = \frac{f_i(x_1, x_2, \ldots, x_j + \varepsilon, \ldots, x_n) - f_i(x_1, x_2, x_3, \ldots, x_j, \ldots, x_n)}{\varepsilon}$$

where

$$\varepsilon = 10^{-5}\lvert x_j\rvert \quad \text{for} \quad \lvert x_j\rvert > 1.0$$
$$\varepsilon = 10^{-5} \quad \text{for} \quad \lvert x_j\rvert < 1.0.$$

Instability may (in many cases) be avoided as follows:

1. Compare the norm of the new function vector to the norm of the previous function vector, where

$$\text{norm} = \sum_{i=1}^{n} \lvert f_i(\tilde{x})\rvert.$$

2. If the norm of the new function vector is greater than that of the old, assume that the full step $\{\delta\}$ would not be productive and take a partial step $\{\delta\}/5$; otherwise, take a full step as usual.

The process of comparing norms and dividing $\{\delta\}$ by an arbitrary constant is termed "damping" and has proved successful in obtaining convergence even with very poor initial guesses.

A weakness of the Newton–Raphson method is that the Jacobian must be calculated at every step.

REFERENCE

1. Suh, C. H., and Radcliffe, C. W., *Kinematics and Mechanisms Design*, John Wiley & Sons, New York, pp. 143–144, 1978.