15BTAR_E29 **COMBUSTION ENGINEERING** **3 0 0 3 100**

OBJECTIVES::

To know the

- Concepts in combustion
- To make combustion calculations
- To know supersonic combustion

UNIT I-FUNDAMENTAL CONCEPTS IN COMBUSTION

Thermo - chemical equations - Heat of reaction first order, second order and third order reactions — premixed flames - Diffusion flames

UNIT II-CHEMICAL KINETICS AND FLAMES

Measurement of burning velocity - Various methods - Effect of various parameters on burning velocity - Flame stability - Detonation - Deflagration - Rankine – Hugoniot curve - Radiation by flames.

UNIT III-COMBUSTION IN GAS TURBINE ENGINES

Combustion in gas turbine combustion chambers - Re-circulation – Combustion efficiency - Factors affecting combustion efficiency - Fuels used for gas turbine combustion chambers - Combustion stability - Flame holder types – Numerical problems.

UNIT IV-COMBUSTION IN ROCKETS

Solid propellant combustion - Double base and composite propellant combustion - Various combustion models - Combustion in liquid rocket engines - Single fuel droplet combustion model - Combustion in hybrid rockets.

UNIT V-SUPERSONIC COMBUSTION

Introduction - Supersonic combustion controlled by mixing, diffusion and heat convection - Analysis of reaction and mixing processes - Supersonic burning with detonation shocks.

TEXTBOOKS:

S.No.	Author(s)	Title of the Book	Publisher	Year of Publication
1.	Samir Sarkar	Fuels and Combustion	Universities Press, North Carolina.	2009
2.	W. H. T. Loh	Nuclear, Ion and Electric Propulsion Theory and Design	Springer, Berlin, Germany.	2012

REFERENCES BOOKS:

S.No.	Author(s)	Title of the Book	Publisher	Year of Publication
1.	Parner, S. F.,	Propellant Chemistry	Reinhold Publishing Corpn, New York	1985.
2.	Gary L. Borman, Kenneth W. Ragland	Combustion Engineering	McGraw Hill, New Delhi.	1998
3.	Kenneth W. Ragland and Kenneth M. Bryden	Combustion Engineering	CRC Press, Florida,United States.	2011

WEB REFERENCES:

- en.wikipedia.org/wiki/**Combustion_Engineering**
- articles.courant.com › Collections
- www.asbestos.com › Asbestos Exposure › Asbestos Manufacturers
- windsorhistoricalsociety.org/fa_**combustion**.html

KARPAGAM ACADEMY OF HIGHER EDUCATION

(Deemed to be University Established Under Section 3 of UGC Act, 1956)

Eachanari post, Coimbatore-641021. INDIA.

FACULTY OF ENGINEERING

DEPARTMENT OF MECHANICAL ENGINEERING

COURSE PLAN

Subject Name : **COMBUSTION ENGINEERING**
Subject Code : **15BTAR7E29** **(Credits - 03)**
Name of the Faculty : **Mrs.P.JAYAPRADHA**
Designation : **ASSISTANT PROFESSOR**
Year/Semester/Section : **III/VI**
Branch : **B.TECH- AEROSPACE ENGINEERING**

Sl. No.	No. of Periods	Topics to be Covered	Support Materials
UNIT I-FUNDAMENTAL CONCEPTS IN COMBUSTION			
1.	1	Basic terms and concepts in combustion	T [1]
2.	1	Fundamental concepts in combustion	T [1]
3.	1	Basic of Combustion Engineering	T [1]
4.	1	Thermo - chemical equations	T [1]
5.	1	Heat of reaction first order reactions	T [1]
6.	1	Heat of reaction Second order reactions	T [1]
7.	1	Heat of reaction Third order reactions	T [2]
8.	1	Premixed flames	T [2]
9.	1	Diffusion flames	T [2]
10.	1	Numerical problems	T [2]
11.	1	**Tutorial- One mark question Test**	
Total No. of Hours Planned for Unit - I			**11**

Sl. No.	No. of Periods	Topics to be Covered	Support Materials
UNIT II-CHEMICAL KINETICS AND FLAMES			
12.	1	Introduction to chemical kinetics and flames	R [5]
13.	1	Measurement of burning velocity	R [5]
14.	1	Various methods of burning velocity	R [5]
15.	1	Effect of various parameters on burning velocity	R [5]
16.	1	Effect of various parameters on burning velocity	R [5]
17.	1	Flame stability	R [5]
18.	1	Detonation and Deflagration	R [5]
19.	1	Rankine Equation	R [5]
20.	1	Hugoniot curve	R [5]
21.	1	Radiation by flames	R [5]
22.	1	**Tutorial – Discussion about Flame stability**	

Total No. of Hours Planned for Unit - II	**11**

Sl. No.	No. of Periods	Topics to be Covered	Support Materials
UNIT III-COMBUSTION IN GAS TURBINE ENGINES			
23.	1	Combustion in gas turbine combustion chambers	R [4]
24.	1	Re-circulation in combustion	R [4]
25.	1	Combustion efficiency	R [4]
26.	1	Factors affecting combustion efficiency	R [4]
27.	1	Fuels used for gas turbine combustion chambers	R [4]
28.	1	Combustion stability	R [4]
29.	2	Flame holder types	R [4]
30.	1	Numerical problems and solutions	R [4]
31.	1	**Tutorial - Small perturbation potential theory**	
Total No. of Hours Planned for Unit - III			**10**

Sl. No.	No. of Periods	Topics to be Covered	Support Materials
UNIT IV-COMBUSTION IN ROCKETS			
32.	1	Introduction to Solid propellant	T [1]
33.	1	Solid propellant combustion	T [1]
34.	1	Double base and composite propellant combustion	T [1]
35.	2	Various combustion models	T [1]
36.	1	Combustion in liquid rocket engines	T [1]
37.	1	Single fuel droplet combustion model	T [1]
38.	2	Combustion in hybrid rockets.	T [1]
39.	1	**Tutorial – One mark Question Test**	
Total No. of Hours Planned for Unit - IV			**10**

Sl. No.	No. of Periods	Topics to be Covered	Support Materials
UNIT V-SUPERSONIC COMBUSTION			
40.	1	Introduction to Supersonic combustion	R [2]
41.	1	Supersonic combustion controlled by mixing	R [2]
42.	2	Supersonic combustion controlled by diffusion	R [2]
43.	1	Supersonic combustion controlled by heat convection	R [2]
44.	2	Analysis of reaction and mixing processes	R [2]
45.	2	Supersonic burning with detonation shocks.	R [2]
46.	1	**Tutorial–One mark questions**	
47.	1	**Discussion on Competitive Examination related Questions / University previous year questions**	
Total No. of Hours Planned for Unit - V			**11**

TOTAL PERIODS :53

TEXTBOOKS:

1. Samir Sarkar, 2009,Fuels and Combustion Universities Press, North Carolina.
2. W. H. T. Loh 2012,Nuclear, Ion and Electric Propulsion Theory and Design Springer, Berlin, Germany.

REFERENCES BOOKS:

1. Parner, S. F., 1985, Propellant Chemistry Reinhold Publishing Corpn, New York
2. Gary L. Borman, Kenneth W. Ragland, 1998 Combustion Engineering McGraw Hill, New Delhi.
3. Kenneth W. Ragland and Kenneth M. Bryden, 2011,Combustion Engineering CRC Press, Florida,United States.
4. Gas Turbine Theory (7th Edition) 7th Edition by H.I.H. Saravanamuttoo (Author), G.F.C. Rogers (Author), H. Cohen (Author), 2017
5. Gas Turbines 3rd Edition by Ganesan, Tata McGraw-Hill Education, 2010.

WEB REFERENCES:

- en.wikipedia.org/wiki/**Combustion_Engineering**
- articles.courant.com › Collections
- www.asbestos.com › Asbestos Exposure › Asbestos Manufacturers

UNIT	Total No. of Periods Planned	Lecture Periods	Tutorial Periods
I	**11**	**10**	**1**
II	**11**	**10**	**1**
III	**10**	**09**	**1**
IV	**10**	**09**	**1**
V	**11**	**09**	**2**
TOTAL	**53**	**47**	**6**

I. CONTINUOUS INTERNAL ASSESSMENT : 40 Marks

(Internal Assessment Tests: 30, Attendance: 5, Assignment/Seminar: 5)

II. END SEMESTER EXAMINATION : 60 Marks

TOTAL : 100 Marks

FACULTY HOD /MECH DEAN / FOE

15BTAR7E16 COMBUSTION ENGINEERING

UNIT I

FUNDAMENTAL CONCEPTS IN COMBUSTION

What is meant by combustion?

- Combustion is a high-temperature exothermic redox chemical reaction between a fuel (the reductant) and an oxidant, usually atmospheric oxygen, that produces oxidized, often gaseous products, in a mixture termed as smoke. Combustion in a fire produces a flame, and the heat produced can make combustion self-sustaining.
- chemical reaction that occurs when oxygen combines with other substances to produce heat and usually light

What is combustion reaction?

A combustion reaction is a type of chemical reaction where a compound and an oxidant is reacted to produce heat and a new product. The general form of a combustion reaction is the reaction between a hydrocarbon and oxygen to yield carbon dioxide and water:

$$\text{hydrocarbon} + O_2 \rightarrow CO_2 + H_2O$$

In addition to heat, it's also common (although not necessary) for a combustion reaction to release light and produce a flame.

In order for a combustion reaction to begin, the activation energy for the reaction must be overcome. Often, combustion reactions are started with a match or other flame, which provides heat to initiate the reaction. Once combustion starts, enough heat may be produced to sustain it until it runs out of either fuel or oxygen.

Combustion Reaction Examples

Examples of combustion reactions include:

$$2\,H_2 + O_2 \rightarrow 2H_2O + \text{heat}$$
$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O + \text{heat}$$

Other examples include lighting a match or a burning campfire.

To recognize a combustion reaction, look for oxygen in the reactant side of the equation and the release of heat on the product side. Because it isn't a chemical product, heat isn't always shown.

Sometimes the fuel molecule also contains oxygen. A common example is ethanol (grain alcohol), which has the combustion reaction:

$$C_2H_5OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$$

A Thermochemical Equation is a balanced stoichiometric chemical equation that includes the enthalpy change, ΔH. In variable form, a thermochemical equation would look like this:

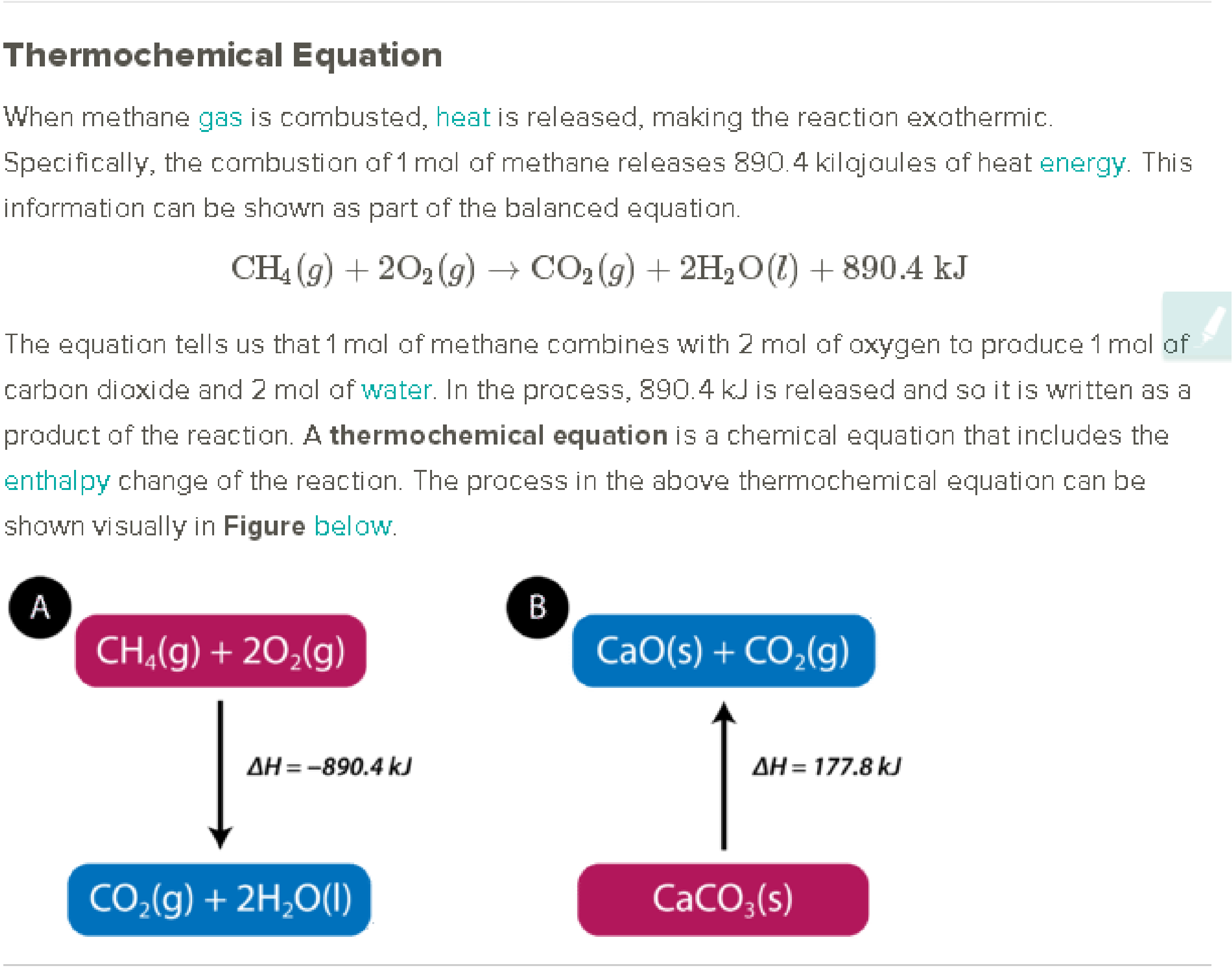
$$A + B \rightarrow C$$

ΔH can have a positive or negative sign. A positive sign means that the system uses heat and is endothermic. The negative value means that heat is produced and the system is exothermic.

$$\text{Endothermic: } A + B + \text{Heat} \rightarrow C,\ \Delta H > 0$$

$$\text{Exothermic: } A + B \rightarrow C + \text{Heat},\ \Delta H < 0$$

Since enthalpy is a state function, the ΔH given for a particular reaction is only true for that exact reaction.

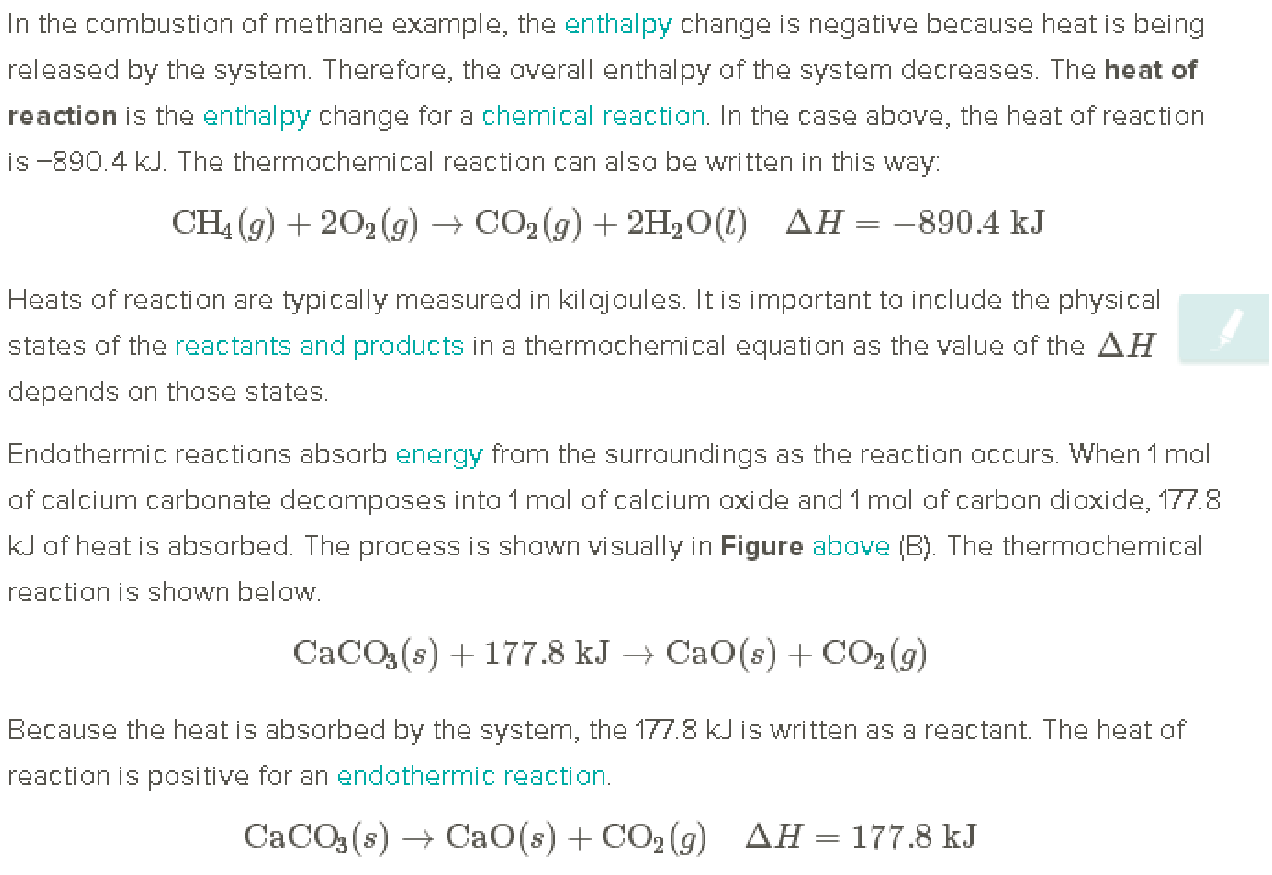


Thermochemical Equation

When methane gas is combusted, heat is released, making the reaction exothermic. Specifically, the combustion of 1 mol of methane releases 890.4 kilojoules of heat energy. This information can be shown as part of the balanced equation.

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l) + 890.4\ \text{kJ}$$

The equation tells us that 1 mol of methane combines with 2 mol of oxygen to produce 1 mol of carbon dioxide and 2 mol of water. In the process, 890.4 kJ is released and so it is written as a product of the reaction. A **thermochemical equation** is a chemical equation that includes the enthalpy change of the reaction. The process in the above thermochemical equation can be shown visually in **Figure** below.



In the combustion of methane example, the enthalpy change is negative because heat is being released by the system. Therefore, the overall enthalpy of the system decreases. The **heat of reaction** is the enthalpy change for a chemical reaction. In the case above, the heat of reaction is −890.4 kJ. The thermochemical reaction can also be written in this way:

$$\mathrm{CH_4}(g) + 2\mathrm{O_2}(g) \rightarrow \mathrm{CO_2}(g) + 2\mathrm{H_2O}(l) \quad \Delta H = -890.4\ \mathrm{kJ}$$

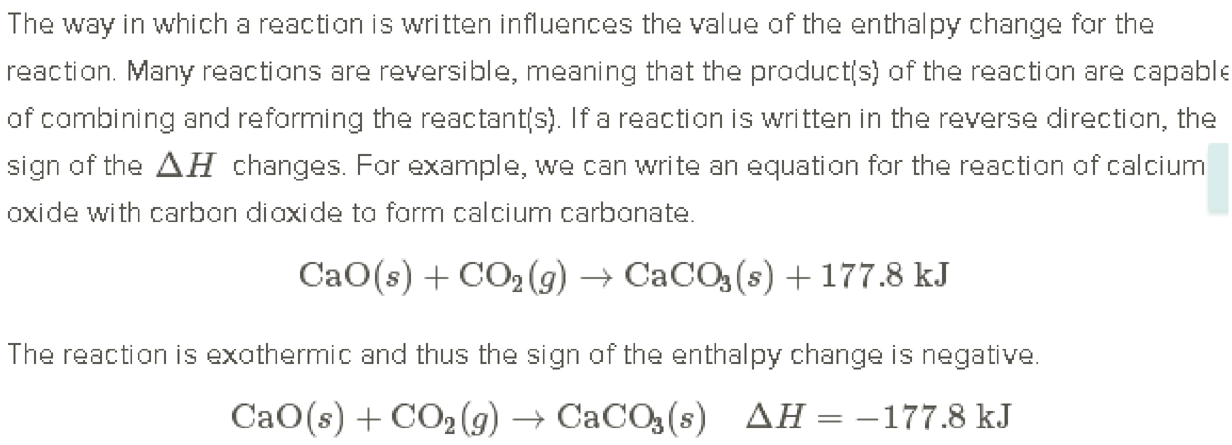
Heats of reaction are typically measured in kilojoules. It is important to include the physical states of the reactants and products in a thermochemical equation as the value of the ΔH depends on those states.

Endothermic reactions absorb energy from the surroundings as the reaction occurs. When 1 mol of calcium carbonate decomposes into 1 mol of calcium oxide and 1 mol of carbon dioxide, 177.8 kJ of heat is absorbed. The process is shown visually in **Figure** above (B). The thermochemical reaction is shown below.

$$\mathrm{CaCO_3}(s) + 177.8\ \mathrm{kJ} \rightarrow \mathrm{CaO}(s) + \mathrm{CO_2}(g)$$

Because the heat is absorbed by the system, the 177.8 kJ is written as a reactant. The heat of reaction is positive for an endothermic reaction.

$$\mathrm{CaCO_3}(s) \rightarrow \mathrm{CaO}(s) + \mathrm{CO_2}(g) \quad \Delta H = 177.8\ \mathrm{kJ}$$



The way in which a reaction is written influences the value of the enthalpy change for the reaction. Many reactions are reversible, meaning that the product(s) of the reaction are capabl of combining and reforming the reactant(s). If a reaction is written in the reverse direction, the sign of the ΔH changes. For example, we can write an equation for the reaction of calcium oxide with carbon dioxide to form calcium carbonate.

$$\mathrm{CaO}(s) + \mathrm{CO_2}(g) \rightarrow \mathrm{CaCO_3}(s) + 177.8\ \mathrm{kJ}$$

The reaction is exothermic and thus the sign of the enthalpy change is negative.

$$\mathrm{CaO}(s) + \mathrm{CO_2}(g) \rightarrow \mathrm{CaCO_3}(s) \quad \Delta H = -177.8\ \mathrm{kJ}$$

What is the thermo chemical equation for the combustion of benzene?

A **thermochemical equation** is simply a balanced chemical equation that includes the change in enthalpy that accompanies that respective reaction.

As is the case with all hydrocarbons, which are compounds that only contain carbon and hydrogen, benzene's combustion will lead to the formation of only two products, carbon dioxide, CO2, and water, H2O.

The balanced chemical equation for the combustion of benzene, C6H6, is

2C6H6(l)+15O2(g)→12CO2(g)+6H2O(l)

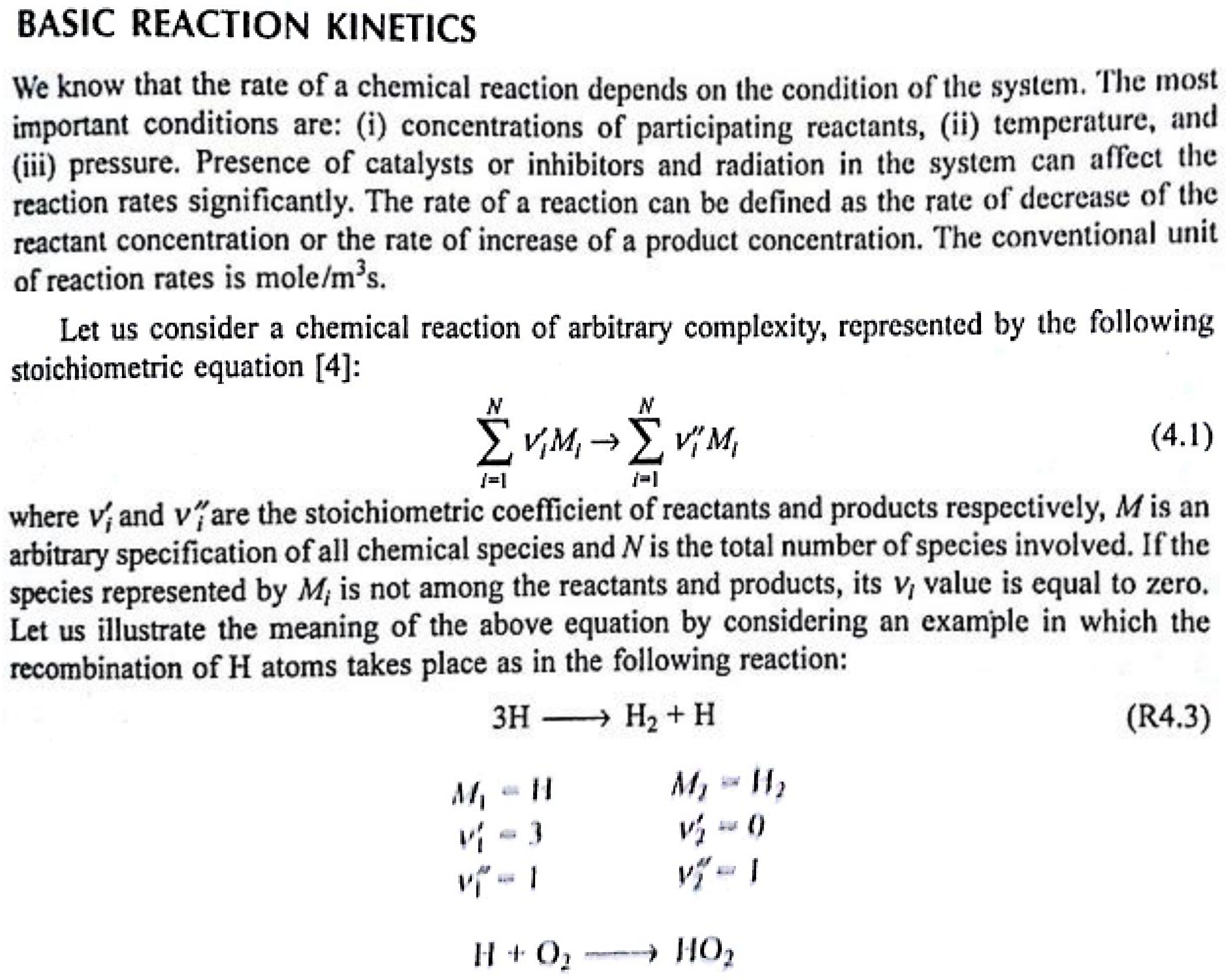
Now, in order to have the **thermochemical equation**, you need to add the change inenthalpy associated with *this reaction*, which is listed as being equal to **-6546 kJ**.

2C6H6(l)+15O2(g)→12CO2(g)+6H2O(l), ΔHrxn=-6546 kJ

You need to be a little careful here because this is the change in enthalpy that accompanies the combustion of **2 moles** of benzene. This means that you can also write

C6H6(l)+15/2O2(g)→6CO2(g)+3H2O(l)
ΔHrxn=-6546/2 kJ=-3273 kJ

This is what the change in enthalpy is when **1 mole** of benzene undergoes combustion.



BASIC REACTION KINETICS

We know that the rate of a chemical reaction depends on the condition of the system. The most important conditions are: (i) concentrations of participating reactants, (ii) temperature, and (iii) pressure. Presence of catalysts or inhibitors and radiation in the system can affect the reaction rates significantly. The rate of a reaction can be defined as the rate of decrease of the reactant concentration or the rate of increase of a product concentration. The conventional unit of reaction rates is mole/m^{3}s.

Let us consider a chemical reaction of arbitrary complexity, represented by the following stoichiometric equation [4]:

$$\sum_{i=1}^{N} \nu_i' M_i \rightarrow \sum_{i=1}^{N} \nu_i'' M_i \qquad (4.1)$$

where ν_i' and ν_i'' are the stoichiometric coefficient of reactants and products respectively, M is an arbitrary specification of all chemical species and N is the total number of species involved. If the species represented by M_i is not among the reactants and products, its ν_i value is equal to zero. Let us illustrate the meaning of the above equation by considering an example in which the recombination of H atoms takes place as in the following reaction:

$$3H \longrightarrow H_2 + H \qquad (R4.3)$$

$M_1 = H$ $\qquad$ $M_2 = H_2$
$\nu_1' = 3$ $\qquad$ $\nu_2' = 0$
$\nu_1'' = 1$ $\qquad$ $\nu_2'' = 1$

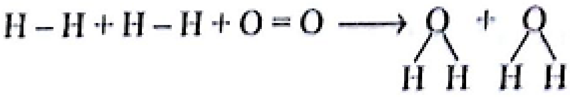
$$H + O_2 \longrightarrow HO_2$$

Note that here, $N = 3$, then

$$\begin{array}{lll} M_1 = H & M_2 = O_2 & M_3 = HO_2 \\ \nu_1' = 1 & \nu_2' = 1 & \nu_3' = 0 \\ \nu_1'' = 0 & \nu_2'' = 0 & \nu_3'' = 1 \end{array}$$

Let us consider an example in which two moles of hydrogen react with one mole of oxygen to produce two moles of water. We can explore this reaction further to appreciate how chemical reaction may occur in reality by using chemical bond format as shown below:

$$2H_2 + O_2 \longrightarrow 2H_2O$$



$$H_2 + H_2 \longrightarrow H + H + H_2$$

HEAT OF REACTION

First Order Reaction

Let us consider a single step first order chemical reaction as given below

$$H_2 \xrightarrow{k_f} 2H$$

The reaction rate would be

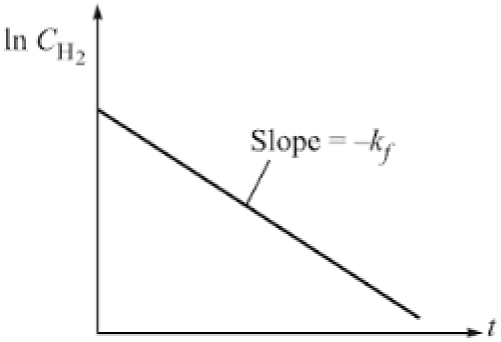
$$-\frac{dC_{H_2}}{dt} = k_f \quad C_{H_2} = \frac{1}{2}\frac{dC_H}{dt}$$

By separating the variables we can integrate the above equation between $t = 0$ and t as given below:

$$-\ln C_{H_2}\Big|_{t=0}^{t=t} = k_f\,(t-0)$$

$$\ln\left(\frac{C_{H_2 0}}{C_{H_2 t}}\right) = k_f\,t$$

This expression indicates that the H_2 concentration decreases exponentially with time as shown in Figure 4.5, when above reaction obeys first order kinetics.



The variation of C_{H_2} with time for a single step first order chemical reaction.

Some of the first order reactions involved during the combustion processes are given below:

$$O_2 \longrightarrow 2O$$

$$N_2O \longrightarrow 2NO_2 + \frac{1}{2}O_2$$

Let us now consider another example in which two molecules, A and B are reacted to produce a single product as given below:

$$A + B \xrightarrow{k_f} C$$

We know that the reaction rate expression is given as

$$\frac{dC_A}{dt} = -\frac{dC_C}{dt} = -k_f\, C_A\, C_B = k' C_A$$

If the concentration of B is quite large as compared to concentration of A, the reaction rate is dependent only on C_A. Then, k' is an apparent specific reaction rate, as C_B remains almost constant. Some of the other complex reactions obeying first order kinetics rate law are thermal decomposition of azomethane, as given below:

$$C_2H_6N_2 \text{ (azomethane)} \rightarrow C_2H_6 + N_2$$

EXAMPLE 4.2 In a first order reaction, $O_2 \longrightarrow 2O$, it was observed that 40% of O_2 is dissociated in 100 s. Determine its specific reaction rate coefficient. What is the half-life of this reaction?

Solution: We know that this first order reaction, $O_2 \longrightarrow 2O$, the reaction rate can be expressed as;

$$-\frac{dC_{O_2}}{dt} = k\, C_{O_2}$$

By separating the variables, we can integrate the above equation between $t = 0$ and t as given below:

$$\ln\left(\frac{C_{O_2,0}}{C_{O_2,t}}\right) = kt$$

where $C_{O_2 \cdot 0}$ and $C_{O_2 \cdot t}$ are the concentrations of O_2 at time $t = 0$ and $t = t$. Then the specific reaction rate coefficient would be expressed as

$$k = \frac{1}{t}\ln\left(\frac{C_{O_2,0}}{C_{O_2,t}}\right) = \frac{1}{100}\ln\left(\frac{100}{60}\right) = 5.1 \times 10^{-3}\ s^{-1}$$

The time required to dissociate O_2 by 50% can be obtained as

$$t = \frac{1}{k}\ln\left(\frac{C_{O_2,0}}{C_{O_2,t}}\right) = \frac{1}{0.0051}\ln\left(\frac{100}{50}\right) = 135.9\ s$$

Second Order Reaction

We know that most chemical reactions are bimolecular in nature. As a result, it is more likely that the chemical reaction often obeys the second order kinetics. The classical example of second order bimolecular reaction is the reaction between H_2 and I_2 to form 2HI, as given,

$$H_2 + I_2 \xrightarrow{k_f} 2HI$$

The reaction rate law for the above reaction becomes;

$$\frac{dC_{H_2}}{dt} = -\, k_f C_{H_2} C_{I_2}$$

We now consider a general second-order reaction as given below:

$$A + B \xrightarrow{k_f} C + D$$

We know that the concentration of species A and B can be expressed as

$$C_A = C_{A,in} - C_X$$
$$C_B = C_{B,in} - C_X$$

where $C_{A,in}$ and $C_{B,in}$ are the initial concentrations of species A and B, respectively and C_X is the concentration portion of species A and B that is consumed during the reaction. Then, the reaction rate law for the above reaction becomes

$$\frac{dC_X}{dt} = k_f\,(C_{A,in} - C_X)\,(C_{B,in} - C_X)$$

Multiplying both the sides of the above equation by $(C_{B,in} - C_{A,in})$ and rearranging, we can get

$$\frac{(C_{B,in} - C_{A,in})\, dC_X}{(C_{A,in} - C_X)(C_{B,in} - C_X)} = k_f\, (C_{B,in} - C_{A,in})\, dt$$

Integrating the above equation between $t = 0$ and t, we can get

$$\int \left(\frac{1}{C_{A,in} - C_X} - \frac{1}{C_{B,in} - C_X} \right) dC_X = \int k_f (C_{B,in} - C_{A,in})\, dt$$

$$\ln \left(\frac{C_{B,in} - C_X}{C_{A,in} - C_X} \right) = k_f\, (C_{B,in} - C_{A,in})\, t + \text{const.}$$

But we know that $t = 0$, $C_X = 0$, then the above equation becomes

$$\ln \left(\frac{C_{B,in}}{C_{A,in}} \right) = \text{const.}$$

Substituting the above expression in Eq. (4.20), we can have

$$\ln \left(\frac{C_{B,in} - C_X}{C_{A,in} - C_X} \right) = k_f\, (C_{B,in} - C_{A,in})\, t + \ln \left(\frac{C_{B,in}}{C_{A,in}} \right)$$

Solving the above equation for k_f, we can get

$$k_f = \frac{1}{t(C_{A,in} - C_{B,in})} \ln \left[\frac{C_{B,in}(C_{A,in} - C_X)}{C_{A,in}(C_{B,in} - C_X)} \right]$$

By using the above equation, we can easily estimate the reaction rate coefficients for second order reactions which will be useful in analyzing the combustion system as most of the chemical reactions involved in the combustion are of second order. Some of the second order reactions involved in the combustion processes are given below:

$$OH + H_2 \longrightarrow H_2O + H$$

$$O_3 + CO \longrightarrow CO_2 + 2O$$

$$O + H_2 \longrightarrow OH + H$$

$$H + O_2 \longrightarrow OH + O$$

$$CH_4 + OH \longrightarrow H_2O + CH_3$$

EXAMPLE 4.3 Hydrogen iodide with initial concentration of 73 mol/m^3 is decomposed to produce H_2 and I_2 molecules as per the following reaction, $2HI \longrightarrow H_2 + I_2$. It is found out that 20% of initial hydrogen iodide is decomposed in 45s. What is the half-life of this reaction? If the initial concentration of hydrogen iodide is doubled, what will be its half-life?

Solution: The reaction rate law for the reaction, $2HI \longrightarrow H_2 + I_2$ becomes

$$\frac{dC_{HI}}{dt} = -k_f C_{HI}^2$$

By separating the variables, we can integrate the above equation between $t = 0$ and t as given below:

$$kt = \frac{1}{C_{HI}} - \frac{1}{C_{HI,0}}$$

where C_{HI_0} and C_{HI_t} are the concentration of HI at time $t = 0$ and $t = t$. Then the specific reaction rate coefficient would be expressed as

$$k = \left(\frac{1}{C_{HI}} - \frac{1}{C_{HI,0}}\right)\frac{1}{t} = \left(\frac{1}{58.4} - \frac{1}{73}\right)\frac{1}{45} = 7.6 \times 10^{-5}\ \text{m}^3/\text{mol}\cdot\text{s}$$

The time required to decompose HI by 50% can be obtained as

$$t = \left(\frac{1}{C_{HI}} - \frac{1}{C_{HI,0}}\right)\frac{1}{k} = \left(\frac{1}{36.5} - \frac{1}{73}\right)\frac{1}{7.6 \times 10^{-5}} = 180.24\ \text{s}$$

When the initial concentration is increased to 146 mol/m^3, the time required to decompose HI by 50% can be obtained as;

$$t = \left(\frac{1}{C_{HI}} - \frac{1}{C_{HI,0}}\right)\frac{1}{k} = \left(\frac{1}{73} - \frac{1}{146}\right)\frac{1}{7.6 \times 10^{-5}} = 90\ \text{s}$$

Third Order Reaction

Let us consider an example of a third order and trimolecular reaction is given below

$$2NO + O_2 \xrightarrow{k_f} 2NO_2$$

The reaction rate law for reaction (R4.24) is given as below:

$$\frac{dC_{NO_2}}{dt} = k_f C_{NO}^2 C_{O_2} = -\frac{1}{2}\frac{dC_{NO}}{dt}$$

This is an overall third order reaction as the reaction rate is proportional to third power of concentration of participating species. Note that reaction rate is strongly dependent on the path. The detailed mechanism of several chemical reactions remains unknown till date as it is quite difficult to measure concentration of species participated significantly during combustion processes. Hence, the thermodynamics state function cannot be used for analysis of chemical reactions occurred during combustion as the rate of reaction is strongly dependent on the path. Some of the third order reactions during combustion are given below:

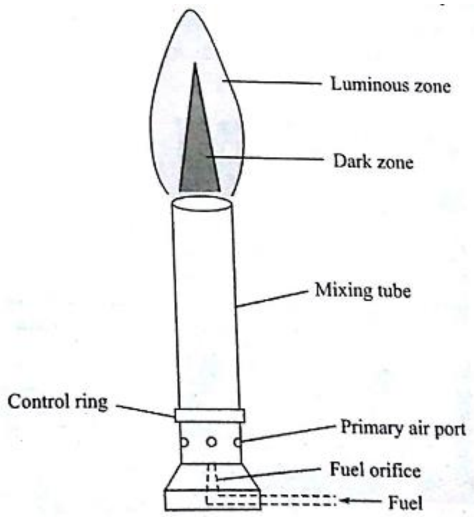
$$H + H + M \longrightarrow H_2 + M \text{ (3rd order)}$$
$$HO + O + M \longrightarrow HO_2 + M \text{ (3rd order)}$$
$$H + H + H \longrightarrow H_2 + H \text{ (3rd order)}$$
$$2NO + O_2 \longrightarrow 2NO_2 \text{ (3rd order)}$$

PREMIXED FLAMES

LAMINAR PREMIXED FLAME

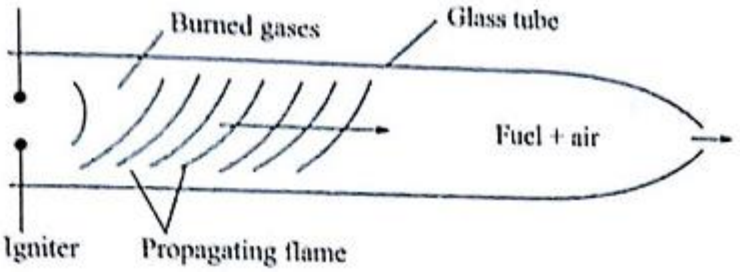
Recently, premixed flames are being employed in many residential, commercial and industrial devices to meet demands made by stringent environmental regulation. Recall that a premixed flame is basically a combustion wave in which fuel and oxidizer are well-mixed beforehand at molecular level. Some of the examples of premixed flames that we come across in our day-to-day life are the flames in the laboratory Bunsen burner, domestic gas burner, heating appliances, jet engine afterburner, etc. It is interesting to note that the first laboratory premixed flame burner was invented by Robert Bunsen way back in 1855.

Let us look at the schematic diagram of a typical Bunsen burner as shown in Figure 5.3 that you must have used previously in the laboratory. In this burner, fuel enters into the burner at its base and is ejected as a jet through a fuel orifice. This fuel jet entrains air into the tube from its surrounding through a number of holes in the burner tube. The fuel and air get mixed thoroughly while flowing up through the tube and become homogeneous mixture by the time they get burnt



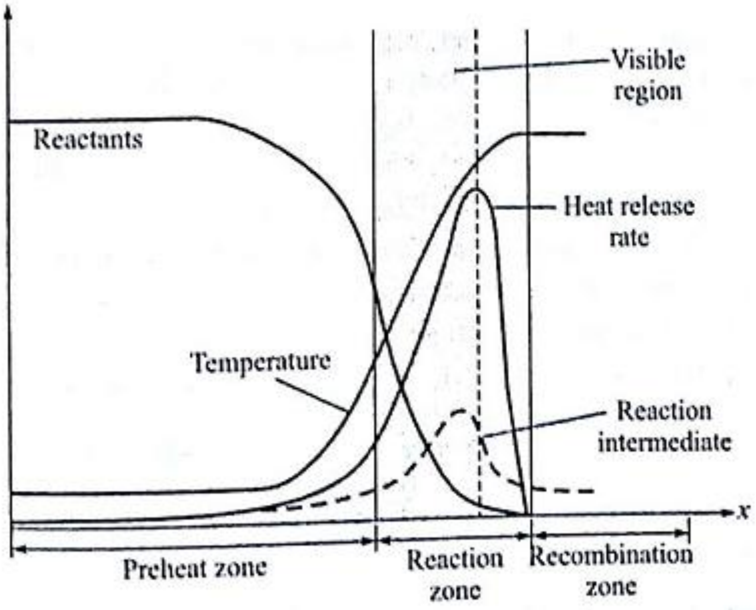
Schematic diagram of a typical Bunsen burner (premixed burner).

The flame structure can be characterized by temperature, heat release and species profiles, as shown in Figure 5.6 for a typical hydrocarbon-air premixed flame. The flame can be divided conveniently into three zones, namely: **(i) preheat zone, (ii) reaction zone,** and **(iii) recombination zone**. The preheat zone is the one in which heat release is negligibly small. However, certain chemical reactions can take place, which prepare the fuel-air mixture to be



Flame propagation in a tube containing flammable fuel-air mixture.

The flame structure can be characterized by temperature, heat release and species profiles, as shown in Figure 5.6 for a typical hydrocarbon-air premixed flame. The flame can be divided conveniently into three zones, namely: **(i) preheat zone, (ii) reaction zone,** and **(iii) recombination zone**. The preheat zone is the one in which heat release is negligibly small. However, certain chemical reactions can take place, which prepare the fuel-air mixture to be



The structure of one-dimensional laminar premixed flame.

Assumptions

(1) One-dimensional steady inviscid flow.

(2) The flame is quite thin. As a result, high temperature reaction zone is restricted to the burnt region of the flame. Hence, major portion of heat release occurs in this zone. The heat release rate is balanced by heat conduction energy equation in this zone.

(3) The ignition temperature, T_{ig} is very close to the flame temperature, T_F.

(4) No heat loss including radiation (adiabatic flame).

(5) The pressure difference across the flame is assumed to be negligibly small. Hence, no need to consider the momentum equation.

(6) Binary diffusion is assumed.

(7) Fourier and Fick's law are valid.

(8) Unity Lewis number $\left(\mathrm{Le}=\frac{\alpha}{D}=1 \Rightarrow \alpha=D\right)$. This simplifies the energy equation.

(9) Constant transport properties such as k_g, C_P, μ, D, etc.

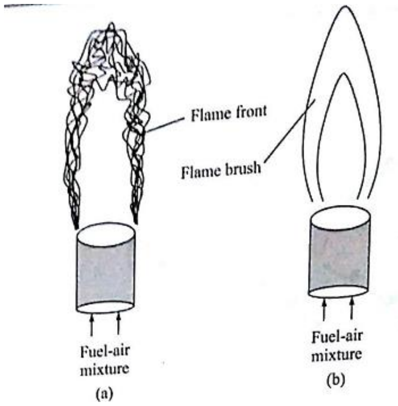
(10) Global reaction mechanism.

Before getting into the analysis of one-dimensional flame, let us consider the structure of steady inviscid one-dimensional premixed flame as depicted in Figure 5.7 for obtaining better

Turbulent Flame Regimes

In a premixed turbulent flame, fuel and oxidizer are being mixed by turbulence during a sufficiently long time before combustion is initiated. The deposition of energy from the spark generates a flame kernel that grows at first by laminar, then by turbulent flame propagation. And in which the oxidizer has been mixed with the fuel before it reaches the flame front. This creates a thin flame front as all of the reactants are readily available. Turbulent flame can be classified into four categories

- Weak turbulent flame
- Wrinkled laminar flame
- Distributed reaction flame
- Flamelet –In–eddy flame



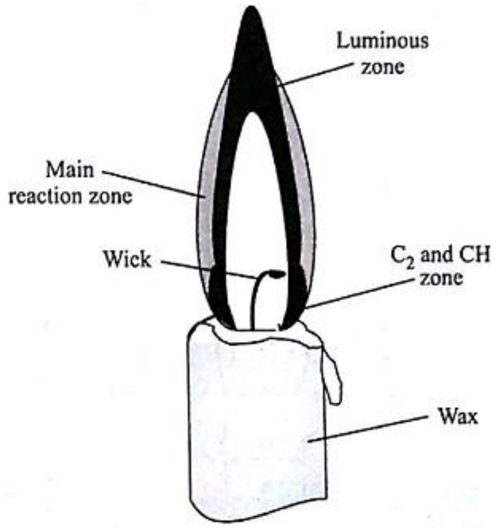
This Reynolds number, Re_l indicates to what extent the larger eddies can be damped by viscosity. The turbulent burning velocity, S_T has been successfully related to Re_l by several researchers [14–19]. Let us now look at another important time scale involved in turbulent flame, which is known as **chemical reaction time**. This can be estimated easily from the laminar flame thickness divided by the laminar burning velocity δ_L/S_L. However, we can define another useful time scale known as **turbulent mixing time scale** based on turn over of eddies. Generally, eddy turn over time can be defined as ratio of largest eddy size, l_0 and rms fluctuating velocity $V'_{\rm rms}$ which can be estimated using largest eddies in the flow. The ratio of turbulent mixing time, t_m (eddy turn over time) and chemical reaction time, t_{ch} is known as **Damköhler number** Da, which is given as

$$Da = \frac{t_m}{t_{ch}} = \frac{l_0/V'_{\rm rms}}{\delta_L/S_L} = \frac{l_0}{\delta_L} \times \frac{S_L}{V'_{\rm rms}}$$

DIFFUSION FLAMES

In combustion, a diffusion flame is a flame in which the oxidizer combines with the fuel by diffusion. As a result, the flame speed is limited by the rate of diffusion.

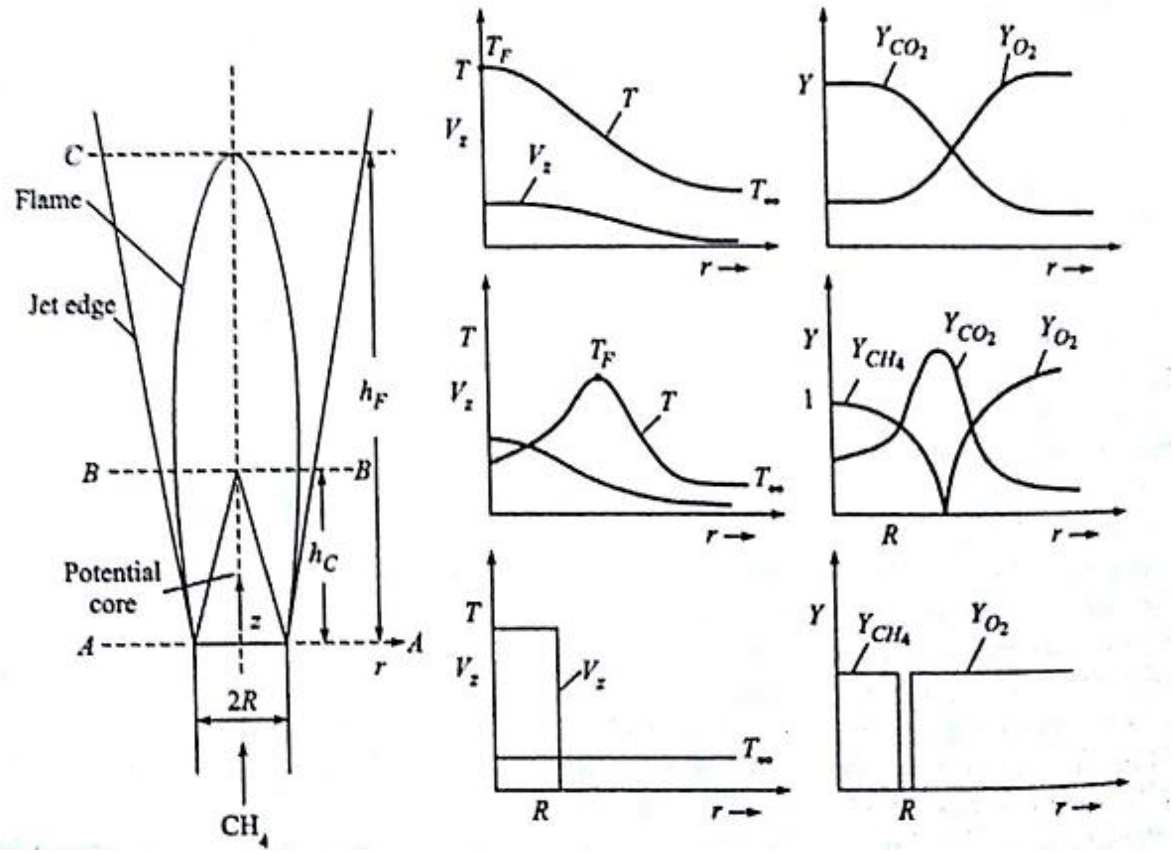
The fuel and oxidizer diffuse to the reaction zones due to molecular and turbulent diffusion and mix at the flame surface itself. As a result, the burning rate is dictated by the rate at which fuel and oxidizer can reach together at the flame surface in proper proportions. Hence, such flame is considered as **diffusion limited**. In contrast, the premixed flame is **kinetically-controlled**, as the reaction rate is most important in deciding the flame structure. Keep in mind that the diffusion flame occurs more often in nature as is the case with the forest fires. When fire is caused in nature, air gets into the flame by diffusion and wind velocity, leading to formation of forest fire.



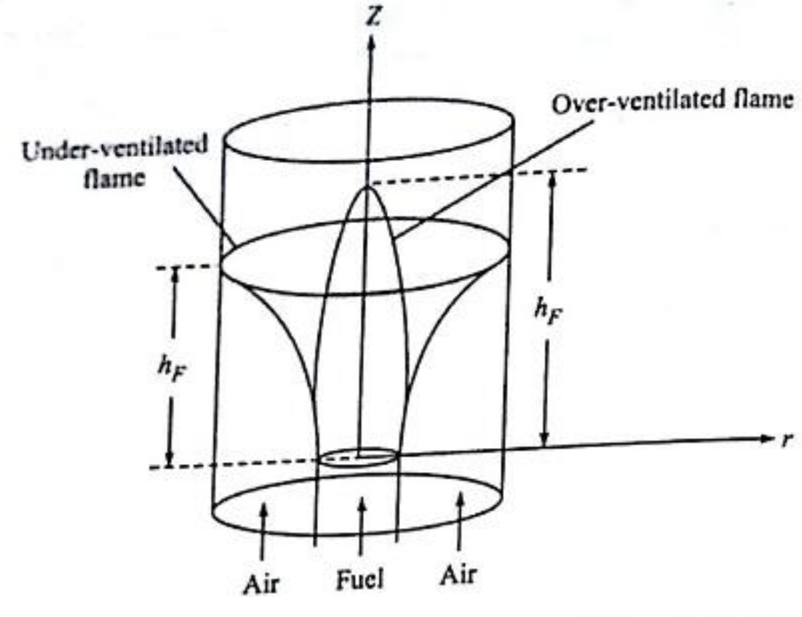
Reaction zones in a candle flame.

Physical Description of Jet Flame

Let us consider a gaseous fuel jet, which is issued from a jet of diameter $D(=2R)$ into quiescent oxidizing atmosphere as shown in Figure 6.2.



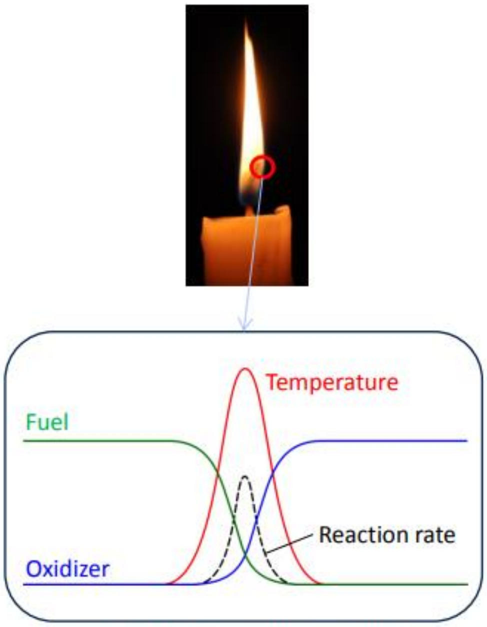
The flame structures of laminar gaseous jet diffusion flame.



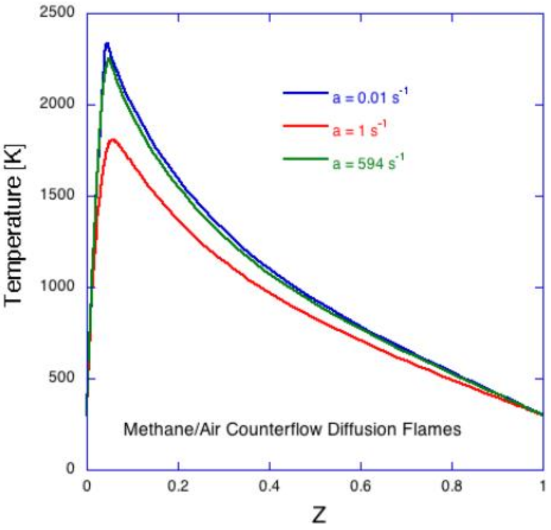
Types of diffusion flame shape: (a) over-ventilated, and (b) under-ventilated.

affected by the mixing rate between fuel jet and oxidizer due to diffusion process. In other words, whenever, fuel and oxidizer come in contact with each other, they react immediately. For a jet diffusion flame, the flame height can be defined as the point along the axis on which inter-diffusion of the fuel and oxidizer is complete at an earliest time. In order words, this is the maximum distance along its jet axis where combustion is complete. At this point, the average depth of penetration of oxidizer into the fuel must be equal to radius of the burner. That means, the end of the flame is reached by a fluid element on the axis in a time magnitude (h_F/V_z), where h_F is the flame height and V_z is the velocity of fuel jet at its inlet. During this time, oxidizer must diffuse into the centre of fuel jet while travelling a distance of radius of burner due to molecular diffusion. We know that the average square displacement ($\bar{r}^2$) due to diffusion as per the **Einstein's diffusion equation** is given by

$$\bar{r}^2 = 2D_{12}t \qquad h_F = \frac{V_z R^2}{2D_{12}}$$



Structure of a diffusion flame (schematic)



UNIT II

CHEMICAL KINETICS

Laminar burning velocity is an important parameter of a combustible mixture as it contains fundamental information regarding reactivity, diffusivity, and exothermicity. Its accurate knowledge is essential for engine design, modeling of turbulent combustion, and validation of chemical kinetic mechanisms. In addition, the determination of burning velocity is very important for the calculations used in explosion protection and fuel tank venting. The burning velocity is defined as the linear velocity of the flame front normal to itself relative to unburned gas, or as the volume of unburned gas consumed per unit time divided by the area of the flame front in which that volume is consumed (Linnett, 1954).

Since the early 1990’s the use of natural gas as an energy source has been increasing rapidly. Natural gas is clean burning and consists of approximately 90 percent methane (CH_4). Due to this high percentage it is important to gain as much knowledge regarding the burning properties and attributes of methane as possible. This project will focus on a mixture of methane and air at various ratios, both greater than and less than stoichiometric. The mixture will be burned to simulate natural gas. The physical property under investigation will be laminar burning velocity.

Laminar burning velocity is highly useful for modeling turbulent burning velocity, (Keck 1982). Turbulent flow occurs when a fluid undergoes irregular fluctuations and mixing. Laminar flow is defined as the flow which travels smoothly in regular paths or layers (Laminar Flow, 2007). According to research by Klimov (1975), the relationship between laminar and turbulent burning velocity can be described by the following equation:

$$\frac{U_T'}{U'} \sim \left[\frac{U_L'}{U'}\right]^{0.3}$$

Equation 1

Where U_T = Turbulent Velocity, U_L = Laminar Velocity. From this equation Klimov concludes that $\frac{U_T'}{U'}$ approaches zero according to the limit $\frac{U_L'}{U'} \to \infty$.

Another instance where laminar burning velocity is used as an input parameter to model a deflagration is the FLACS Code, developed by GexCon. The FLACS Software Suite is primarily used to model various types of explosions. Specifically, laminar burning velocity is used in the FLACS model for combustion. The model assumes that an explosion can be represented by many small flamelets, which can be considered laminar. Laminar burning velocity models are one of the three input parameters for this program and they are a function of the gas mixture, temperature, and pressure. The second input parameter is a turbulent burning velocity model, which depends upon numerous turbulence parameters, and is determined through experimental data. The final parameter quantifies a model describing quasi-laminar combustion shortly after ignition of the flame, (GexCon, 2007).

There are many experimental techniques used in obtaining the laminar burning velocity of a particular gas-air mixture. A critical review of these methods is available in the literature

(Andrews and Bradley, 1972). Apparatuses for measuring laminar burning velocity can be classified into two categories: constant volume and constant pressure. Examples of these are the spherical bomb technique for constant volume, and the slot-burner for constant pressure. The key differences are the ranges of pressure and temperature that can be included in the tests. The constant pressure methods primarily use atmospheric pressure, and approximately constant temperatures, while the constant volume methods can measure burning velocity under a wide range of temperatures and pressures (Parsinejadet et al., 2006). This project uses the slot-burner and Bunsen burner technique to calculate the flame velocities. The slot burner is chosen due to its advantages involved in the theory of the velocity calculation as well as ease of apparatus construction. The burning velocity obtained using the slot burner method is calculated by multiplying the gas mixture flow rate by the sine of the flame angle.

$$S_u = U\sin\alpha$$

Equation 2

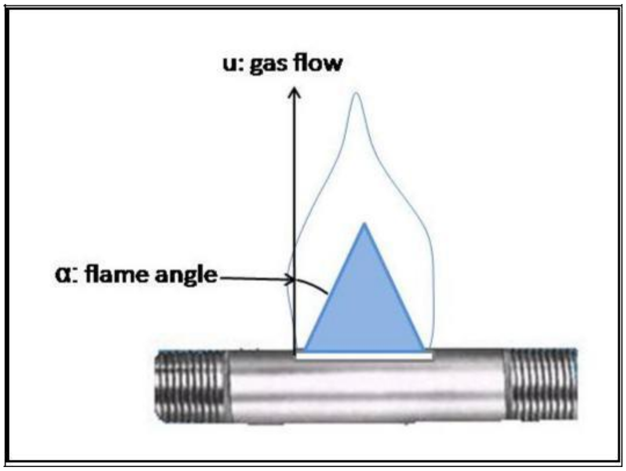


Figure 1: Illustration of experimental parameters used to calculate burning velocity using the slot burner method.

The Bunsen burner apparatus is decided upon because it should provide data that is accurately comparable to previously published data. The Bunsen burner uses the flame surface area and total flow of gas to calculate the laminar burning velocity.

$$v_b = \frac{\text{input volumetric flow}}{\text{total flame area}}$$

Equation 3

The flame produced in both apparatuses is stabilized and adjusted to provide the most uniform, symmetrical flame possible. This is done by increasing or decreasing the flow of fuel and air. The flame will then be photographed using a high resolution camera. Finally, from the pictures of the flames the flame angles and heights will be measured and then the burning velocity will be calculated.

There are a variety of techniques used to measure laminar burning velocity. This section discusses a few of these methods .

Description: A flame is stabilized over a rectangular opening. A Mache-Hebra (or similar) nozzle

Advantages	**Disadvantages**
Flame has large flat areas in which curvature is minimized	Angle α is difficult to measure accurately

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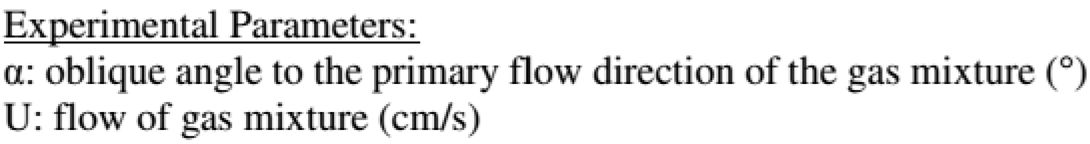
Flame has large flat areas in which curvature is minimized	Angle α is difficult to measure accurately

Experimental Parameters:



Experimental Parameters:

α: oblique angle to the primary flow direction of the gas mixture (°)

U: flow of gas mixture (cm/s)

Formula:

$S_u = U\sin\alpha$ (Strehlow 1984)

S_u: Burning velocity (cm/s)

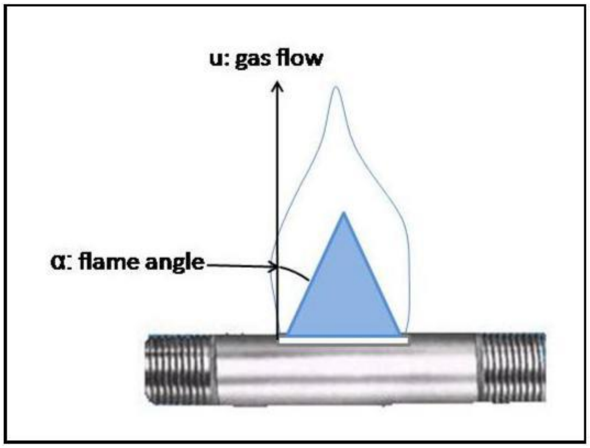


Figure 2: Illustration of Experimental Parameters used to calculate Burning Velocity

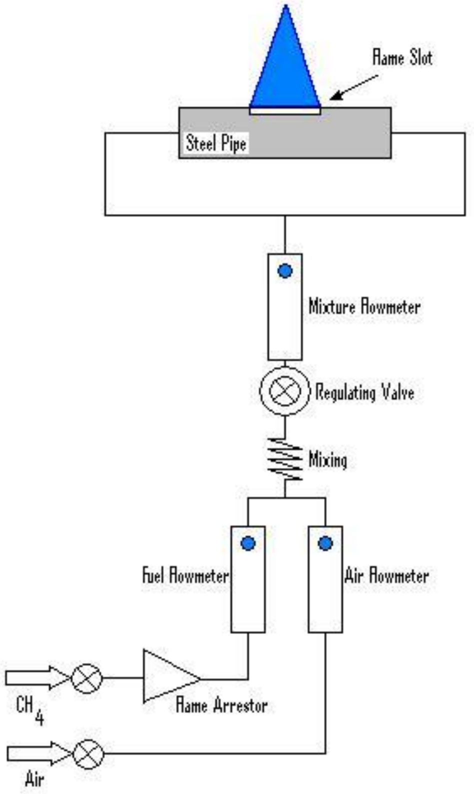


Figure 3: Design of Slot Burner Apparatus

Bunsen Burner Method

Description: Most commonly performed using a Bunsen burner, the flame surface area is simply measured and divided by the amount of gas mixture consumed per second. There are many ways to perform this experiment; however, it is not known which method is the most accurate, (Vagelopoulos 1998).

- Particle track method
- "Frustrum" Method- Lewis and Von Elbe (base and tip are not included in flame area)
- Angle method with Schlieren cone

Flame Shape: Varying

Advantages	Disadvantages
Simple apparatus It is also possible to test the effects of temperature and pressure	Low accuracy Unreliable theory Only avg burning velocity can be obtained Complex flame shapes Not possible with very fast flames

Experimental Parameters:

Volumetric flow (cm^3/s)
Area of flame (cm^2)

Formula:

$$v_b = \frac{input\ volumetric\ flow}{total\ flame\ area}$$

v_b: Burning Velocity (cm/s)

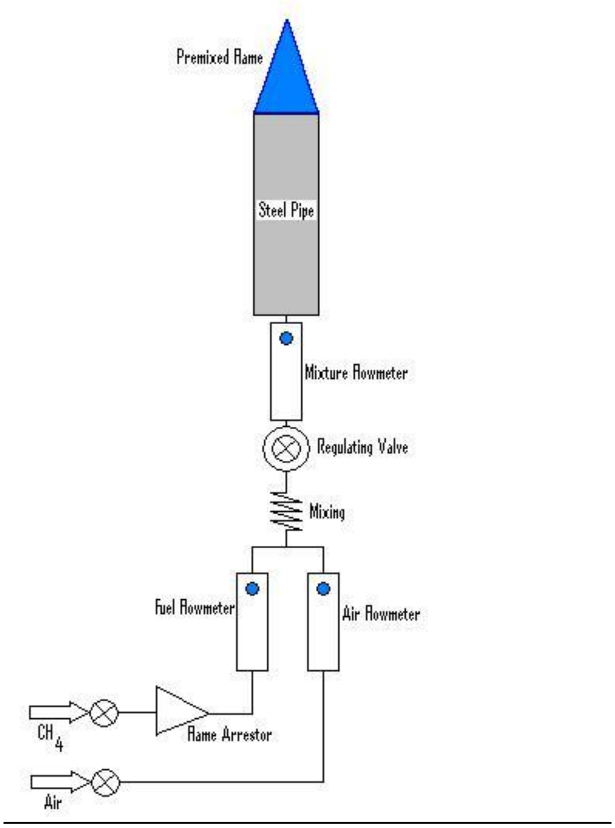


Figure 4: Typical Bunsen Burner

Tube Propagation Method

Description: A horizontal tube is filled with a gas mixture. One end of the tube is open, the other closed. A flame is ignited at the open end of the tube and a series of snapshots records the flame as it travels down the length of the tube.

Flame Shape: Hemispherical or Ellipsoidal

Advantages	**Disadvantages**
Small quantities of materials needed	Cooling effect of walls create errors
Widely applicable	Measurement of flame area is difficult
Simple apparatus	Only an avg burning velocity can be obtained

Experimental Parameters:

A: area of flame (cm^2)

v_m: speed of flame (cm/s) $\left(\frac{Lengthoftube(cm)}{Timeittakesflametotravelentirelengthoftube(sec)}\right)$

Formula:

$$v_b = \frac{v_m \pi R_2}{A}$$ (Linnett 1954)

V_b = Burning velocity (cm/s)

R_2 = Radius of tube (cm)

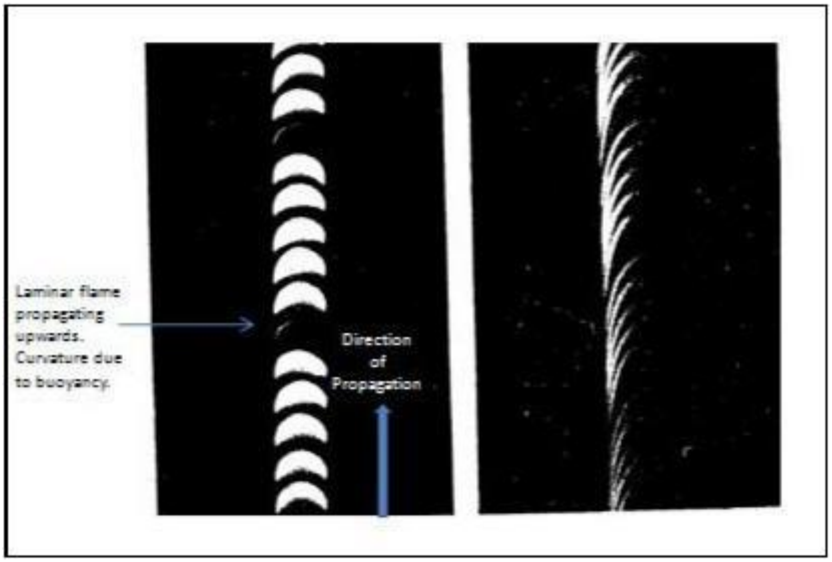


Figure 5: Snapshots of two flames as they propagate along a tube filled with two different fuel types. The picture on the right shows a fuel with a higher burning velocity than that of the picture on the left. This is determined by the spacing between each arc.

Soap Bubble Technique

Description: A soap bubble is blown with gas mixture and a capacitance spark ignites the flame within the bubble. It then burns as an outwardly propagating spherical flame. The flame is photographed using a rotating drum camera. The initial and final diameters are measured for the expansion ratio.

Flame Shape: Spherical

Advantages	Disadvantages
Simple interpretation because explosion occurs at constant temperature Small quantities of materials needed Flame is simple spherical form (spherical)	Gas may diffuse through soap bubble Soap can add water to gas mixture Measuring final bubble diameter is difficult Flames may not retain spherical shape Will not work with slow flames because convection will destroy spherical flame shape

Experimental Parameters:

r_1: Initial radius of soap bubble (cm)
r_2: Final radius of soap bubble (cm)

Formula: $S_u = \left(\frac{r_1}{r_2}\right)^3 S_b$ (Streholow 1984)

S_b: Volumetric flow (cm^3/s)
S_u = Burning velocity (cm/s)

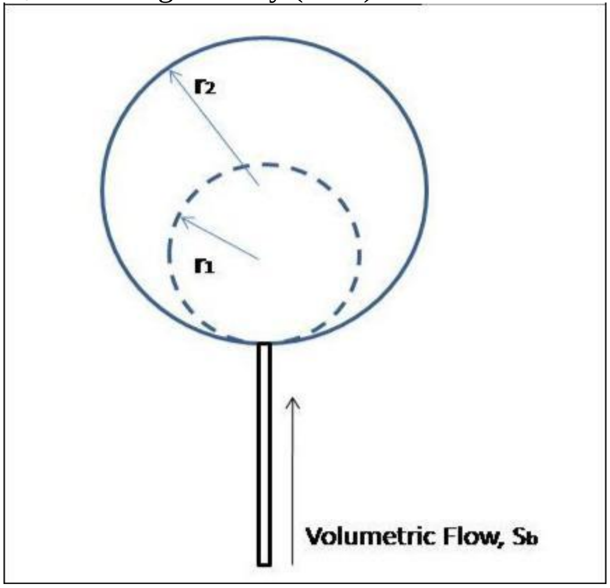


Figure 6: Variables involved in soap bubble technique equation

Constant Volume Explosion in Spherical Vessel

Description: Gas mixture is ignited at the center of a spherical bomb.

Flame Shape: spherical

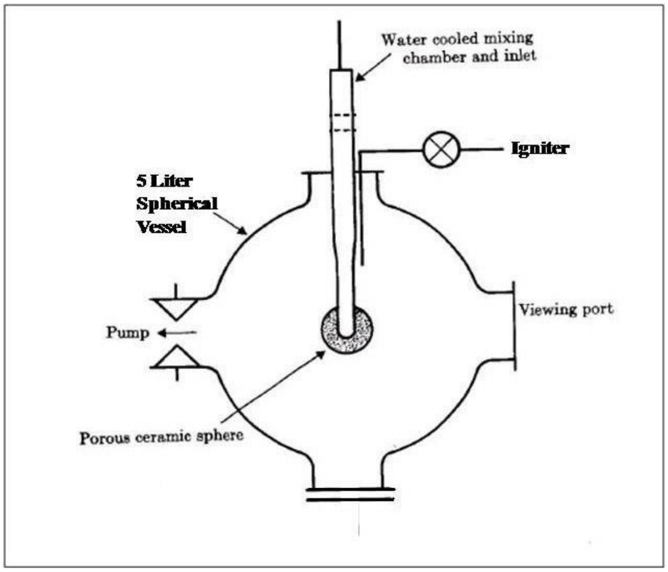
Advantages	Disadvantages
Simple flame shape	Pressure is inconstant
Small quantities of materials needed	Flame may not remain spherical
Widely applicable	Complicated apparatus
	Theory is uncertain

Experimental Parameters:
p: pressure at time t (Pa)
r: flame radius at time t (cm)

Formula:

$$v_b = \left[1 - \frac{R^3 - r^3}{3p\gamma r^2}\frac{dp}{dr}\right]\frac{dr}{dt} \quad \text{(Linnett 1954)}$$

V_b = Burning velocity (cm/s)



Flat Flame Burner

Description: A low velocity flow of the gas mixture is passed through a series of screens and honeycomb filters to create an even, flat flame, (Gaydon 1970).

Flame Shape: Flat

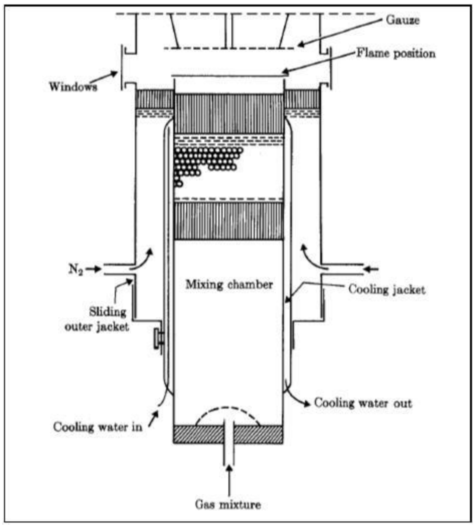
Advantages	Disadvantages
Flat flame profile most closely approaches an infinite plane Useful for mixtures nearing the limits of flammability	Can only be used for slow flames (<15cm/sec) Matrix heats up (sometimes up to 200°C) and preheats gas mixture

Experimental Parameters:
Flame area (cm^2)
Volumetric flow rate (cm^3/s)

Formula:

$$v_b = \frac{\text{input volumetric flow}}{\text{total flame area}}$$ (Gaydon 1970)

V_b = Burning velocity (cm/s)



The slot burner method is chosen for measuring burning velocity for two specific reasons. First, the theory is relatively simple. Burning velocity is calculated by multiplying the gas flow rate by the sine of the acute angle between the direction of gas flow and the flame edge. The second reason for choosing this method is that the apparatus is relatively simple to construct and can be created by satisfying a small number of specifications. The first requirement being that the air and methane must be pre-mixed within the apparatus. Secondly, the gas mixture must exit through a slot of ratio 3:1 (length to width) or greater. Lastly, it is important that the apparatus be capable of creating and maintaining a steady flame characterized by a defined inner triangle.

Air for the experiment is delivered via an in-house compressed air system. A line of steel braided tubing joins this delivery system to the slot burner itself. The methane is stored in a compressed cylinder located approximately one meter away from the apparatus. Another steel braided tube delivers the methane supply to a separate branch of the slot burner, after passing through a methane-rated flame arrestor. Each of these supply sources is equipped with a regulator as well as a pressure gage. The air then passes through a flow meter of scale 7-70 standard cubic feet per hour (SCFH). The methane passes through a flow meter of scale 1-11 SCFH. These flow meters are used for the purpose of identifying the resulting gas mixture composition. The supplies then flow through approximately 30 cm (equidistantly) to a T-union where they simultaneously flow into a 5.2cm (3 in) diameter clear plastic tube. This tube is filled with glass beads of diameter 6mm (0.326 in) meant to mix the air and methane into an approximately uniform distribution. The newly mixed gas then passes through a regulator valve. The purpose of this valve is to manage the flow exiting the slot thereby reducing turbulence. This is followed by a third flow meter of scale 7-70 SCFH to measure the actual gas flow exiting the slot burner. This value is used in calculation of the burning velocity. The gas mixture is then split once again at a T-union and delivered via PVC tubing to opposite ends of a 1.27 cm (½ in) diameter, 15.24 cm (6 in) long steel pipe. The inner wall of which has a fine mesh used to pressurize flow within the pipe, thereby reducing turbulence through the slot which is located at the top center of the pipe.

Only a few alterations are made in order to convert the slot burner design to a Bunsen burner design. For the first test a 1.524cm diameter by 30.48cm long (1/2” x 12”) pipe is oriented vertically directly above the regulator valve. This way the flow no longer splits into two directions and exits directly at the top of the steel pipe where the laminar flame forms. Experimental parameters measured are the height and base of the flame as well as the volumetric flow exiting the pipe. Other burner diameters tested are 0.76cm and 1.016cm. The burning velocity is found by dividing the volumetric flow by the area of the flame.

A leakage test is performed before every experiment to minimize the risk of a methane leak. This is done by first opening the air supply line and applying a leak identifying agent (Snoop) to every point with the potential for leakage. Connections are tightened until bubbles caused by Snoop are no longer present. The same process is completed along the methane line. A flame is lit at the top of the apparatus during this time to ensure that the methane is consumed rather than let out into the atmosphere.

Flame Stabilization :

The velocities encountered in modern propulsion engines and power plant burners are so high that the flame has to be stabilized by some artificial means.

Considering blow-off as a situation arising to allow the residence time of the reactions to proceed to ignition, one may devise various possible flame stabilizers.Velocity is slowed down, flow remains high.

There are 3 types of flame stabilizers are extensively known. They are:

Stabilization by Pilot Flames
by Bluff Bodies and
by Recirculation

By Pilot Flames

Suppose a pilot flame (as hot inert gas in Fig 8.28) is held adjacent to the cold reactant mixture flow issuing in the form of a high velocity jet.

Heat and mass are transferred across the boundary of the two streams by diffusion and mixing.

The reaction rate in the cold reactant mixture is thus enhanced shown in Figure 8.28 (Marble and Adamson).

Blow-off would occur if the flow rate > the reaction rate in reactant mixture.

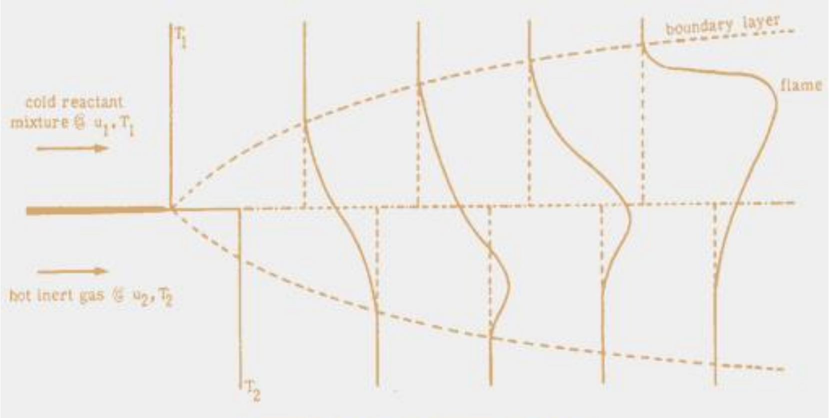


Figure 8.28 The Marbel-Adamson problem

By Bluff Bodies

When a blunt body is placed in a high velocity reactant stream, the flow is greatly slowed down at the forward stagnation point (see Figure 8.29) to give ample opportunity for reactions to proceed to ignition.

One major disadvantage of solid bluff bodies is the drag they exert on the flow and the resultant loss of thrust.

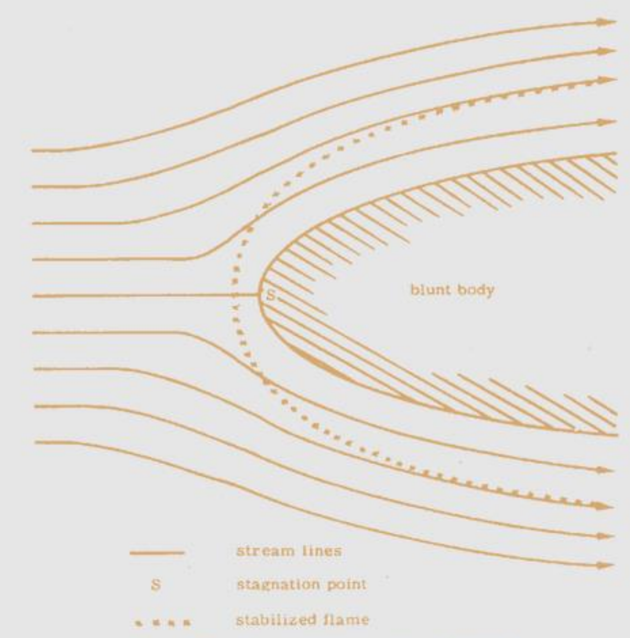


Figure 8.29 Flame stabilization by a blunt body

Campbell overcomes this drawback by employing an opposing gaseous jet in the reactant stream.

It evolves as the opposing jet. The stream is slowed down and the flame is anchored as schematically shown in Figure 8.30. The blow-off velocity is increased by increasing the injection pressure of the opposing jet and by increasing the temperature of the opposing jet gas.

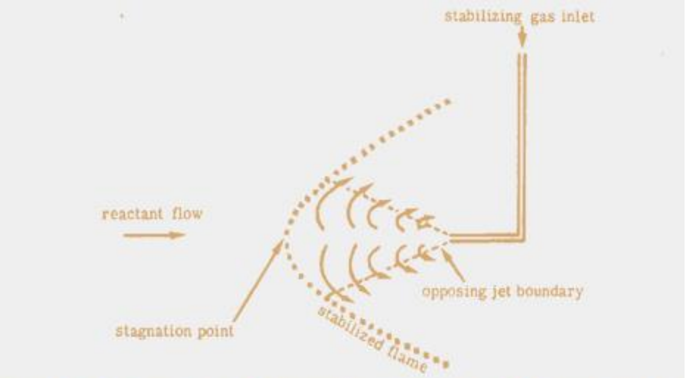


Figure 8.30 Flame stabilization by an opposing jet (adapted from: A. B. Campbell and B. H. Jennings, *Gas Dynamics*, McGraw-Hill, (1958))

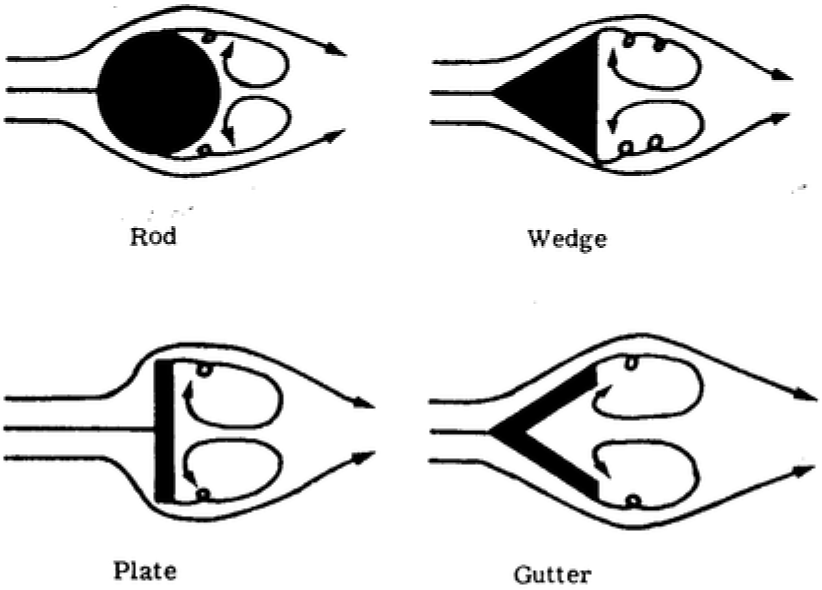
By Recirculation

When the solid bluff body discussed above is of finite length in the direction of flow, the pressure distribution prevents the high velocity flow from keeping attached to the solid surface.

Increasing pressure separates the boundary layer and causes eddy shedding in the "wake."

Under sufficiently fast flow conditions a (symmetric) recirculation pattern of flow is established behind the blunt body as shown in Figure 8.31.

The recirculation zone provides a station where reactions can take place.



Rod

Wedge

Plate

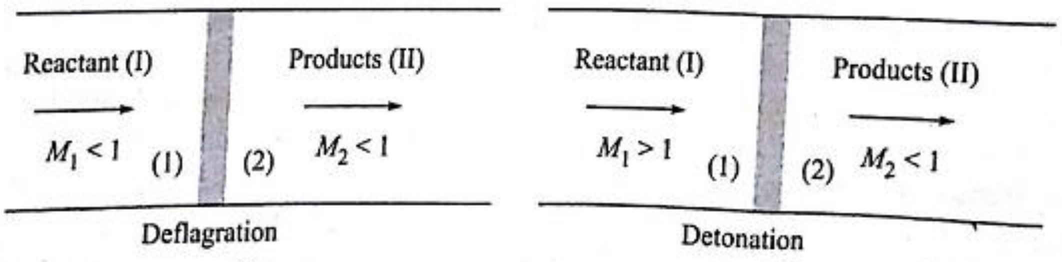
Gutter

Figure 8.31 Flame stabilization by recirculation

ONE-DIMENSIONAL COMBUSTION WAVE

Let us consider a long tube, which contains combustible gaseous fuel-oxidizer mixture. If ignition energy is supplied at one end, a combustion wave will propagate downstream of the tube towards unburnt mixture. When the tube is open at both ends, combustion waves move at a speed in the range of 20–340 cm/s depending on the type of fuel-air mixture and equivalence ratio prevailing in the tube. It must be appreciated that velocity of combustion wave is much less than the speed of sound. In this case, transport processes involving simultaneous conduction of heat and diffusion of radicals govern the speed of combustion wave. Recall that the combustion wave is generally known as **flame** and if the velocity of flame is subsonic, this is termed as **deflagration** (Figure 5.1a).

Now, if the tube containing fuel-air mixture is closed at both ends and is ignited, the combustion wave undergoes a transition from subsonic to supersonic speed. Such a kind of combustion wave is known as **detonation**. Speed of detonation is not controlled by heat conduction and radical diffusion like deflagration. Rather, the shock wave causes the temperature and pressure to increase to such a great extent that it can lead to explosion and large amounts of energy is released during this process. Both subsonic and supersonic waves can be obtained under similar condition. Let us learn more about it by considering this interesting phenomenon without considering chemical reactions. For this analysis, we can consider a steady one-dimensional flow with external heat transfer as shown in Figure 5.1. Let us then presume that a chemical reaction coupled with a normal shock undergoes a transition from state (I) to (II) as shown in Figure 5.1(b).



Deflagration
(a)

Detonation
(b)

$$\text{Continuity: } \rho_1 V_1 = \rho_2 V_2 = \dot{m} = \text{constant}$$
$$\text{Momentum: } P_1 + \rho_1 V_1^2 = P_2 + \rho_2 V_2^2$$
$$\text{Energy: } C_{P_1} T_1 + \frac{V_1^2}{2} + q = C_{P_2} T_2 + \frac{V_2^2}{2}$$
$$\text{State: } P_1 = \rho_1 R T_1$$
$$\text{State: } P_2 = \rho_2 R T_2$$

where ρ, V, P, T are the density, velocity, pressure and temperature, respectively, q is the heat release per unit mass equal to $\sum Y_i \Delta h^0_{f,i}$, Y_i is the mass fraction of i^{th} species and $\Delta h^0_{f,i}$ is the heat of formation of i^{th} species. For simplicity, we have assumed perfect gas at stations (1) and (2) as evident in Eqs. (5.4–5.5). Note that Eq. (5.5) is not an independent equation as this is related to unknown variables, such as unburned gas pressure, temperature and density. In the chosen coordinate system, V_1 is the velocity of fuel-oxidizer mixture fed into the wave, V_2 is the velocity away from the wave. However, in the laboratory coordinate system, the velocity V_1 which is ahead of wave, is equal to zero. Thus, $(V_1 - V_2)$ is the speed of the burned gases with respect to the tube. We need to evaluate five unknowns such as V_1, V_2, P_2, T_2 and ρ_2, using only four independent equations (Eqs. 5.1–5.4). We now wish to convert these four independent equations to a single equation with two unknowns, i.e., P_2 and ρ_2. Combining continuity equation (Eq. 5.1) and momentum equation (Eq. 5.2), we can have

$$P_2 - P_1 = \rho_1 V_1^2 - \rho_2 V_2^2 = \frac{(\rho_1 V_1)^2}{\rho_1} - \frac{(\rho_2 V_2)^2}{\rho_2} = \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)\dot{m}^2$$

$$\rho_1^2 V_1^2 = \frac{P_2 - P_1}{\left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)} = \dot{m}^2$$

Equation (5.7) is known as the **Rayleigh relation.** This can be expressed in terms of Mach number $M_1 = V_1/c_1$, (c_1 = speed of sound = $\sqrt{\gamma(P_1/\rho_1)} = \sqrt{\gamma R T_1}$). Then, Eq. (5.7) becomes

$$V_1^2 = \frac{(P_2 - P_1)}{\rho_1^2\left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)}$$

Then,
$$M_1^2 = \frac{V_1^2}{\gamma P_1/\rho_1} = \frac{1}{\gamma}\left(\frac{P_2/P_1 - 1}{1 - \rho_1/\rho_2}\right) \tag{5.8}$$

Similarly, we can have an expression for downstream velocity, V_2 by using Eqs. (5.1) and (5.2) as given below

$$V_2^2 = \frac{1}{\rho_2^2}\frac{(P_2 - P_1)}{\left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)} \tag{5.9}$$

The above equation can also be expressed in terms of Mach number as given below

$$\frac{V_2^2}{\gamma P_2/\rho_2} = M_2^2 = \frac{1}{\gamma}\left(\frac{1-P_1/P_2}{\rho_2/\rho_1-1}\right)$$

Let us express q in the energy equation (Eq. 5.3) in terms of P, ρ, V considering the gas to behave as a perfect gas. But we know that for a perfect gas

$$\gamma = \frac{C_P}{C_v}; \quad C_P T = \frac{\gamma}{\gamma-1}\frac{P}{\rho}$$

Using these relations in the energy equation (Eq. 5.3), we can get

$$q = \frac{\gamma}{\gamma-1}\left(\frac{P_2}{\rho_2}-\frac{P_1}{\rho_1}\right)+\frac{1}{2}(V_2^2-V_1^2)$$

$$q = \frac{\gamma}{\gamma-1}\left(\frac{P_2}{\rho_2}-\frac{P_1}{\rho_1}\right)-\frac{1}{2}(P_2-P_1)\left(\frac{1}{\rho_1}+\frac{1}{\rho_2}\right)$$

Equation (5.13) is known as the **Rankine-Hugoniot relation**.

This Rankine-Hugoniot relation is one of the most important relations for both deflagration and detonation waves and can be used for both flame and explosion phenomena. When there would not be any heat release ($q = 0$) due to chemical reactions, this relation can describe the normal shock wave. The variation of P_2 is plotted against $1/\rho_2$ for a fixed value heat release per unit mass q, inlet pressure P_1 and inlet density $1/\rho_1$, which is known as **Hugoniot curve** as shown in Figure 5.2.

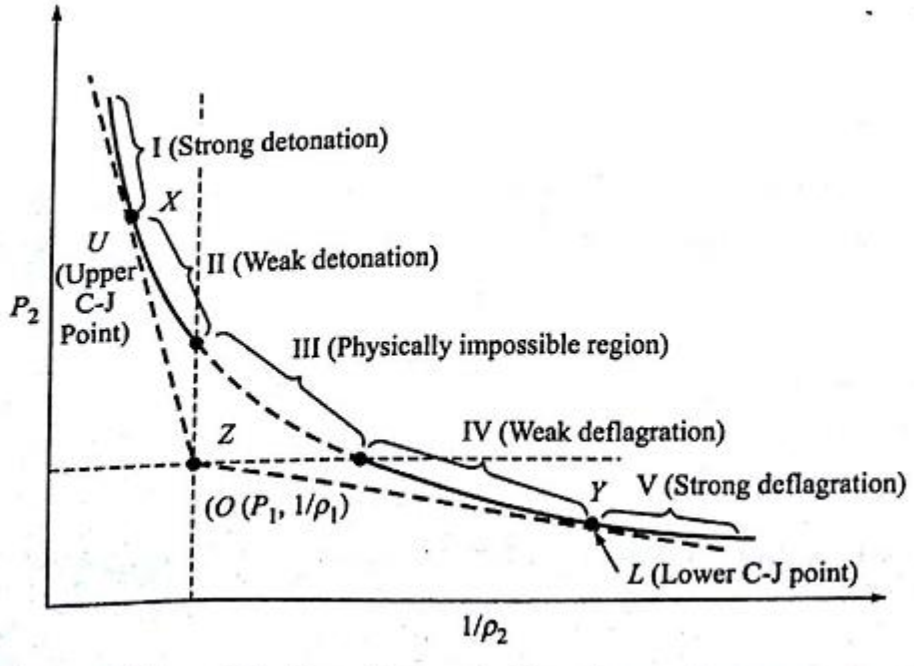


Figure 5.2 Hugoniot curve with various regimes.

RADIATION BY FLAMES.

Combustion consists of chemical reactions in series and in parallel and involving various intermediate species. The composition and concentration of these species cannot be predicted very well unless knowledge is available of the flame reaction kinetics; this detailed knowledge is not usually available or convenient to obtain. Because the flame radiation properties depend on the distributions of temperature and species within the flame, a detailed prediction of radiation from flames is not often possible from knowledge of only the combustible constituents and the flame geometry. It is usually necessary to resort to empirical methods for predicting radiative transfer in systems involving combustion.

Radiation from the non luminous portion of the combustion products is fairly well understood. For this the complexities of the chemical reaction are not as important, since it is the gaseous end products above the active burning region that are considered. Most instances are for hydrocarbon combustion, and radiation is from the CO_2 and H_2O absorption bands in the infrared. For flames a meter or more thick, as in commercial furnaces, the emission leaving the flame within the CO_2 and H_2O vibration-rotation bands can approach blackbody emission in the band spectral regions. The gas radiation properties in Chap. 9, and the methods in this chapter, can be used to compute the radiative transfer.

The analysis is greatly simplified if the medium is well mixed and can be assumed isothermal. A non isothermal medium can be divided into approximately isothermal zones, and convection can be included if the circulation pattern in the combustion chamber is known.

Radiation from various types of non luminous flames (laminar or turbulent, mixed or diffusion) is treated. The flame shape for an open diffusion flame is considered in Annamali and Durbetaki (1975). The local absorption coefficient in non luminous flames is calculated in Grosshandler and Thurlow (1992) as a function of mixture fraction and fuel composition. Modest (2005) reviews models for radiative transfer in combustion gases.

When considering the radiation from flames, a characteristic parameter is the average temperature of a well-mixed flame as a result of the addition of chemical energy. Well-developed methods exist for computing the theoretical flame temperature from thermodynamic data.

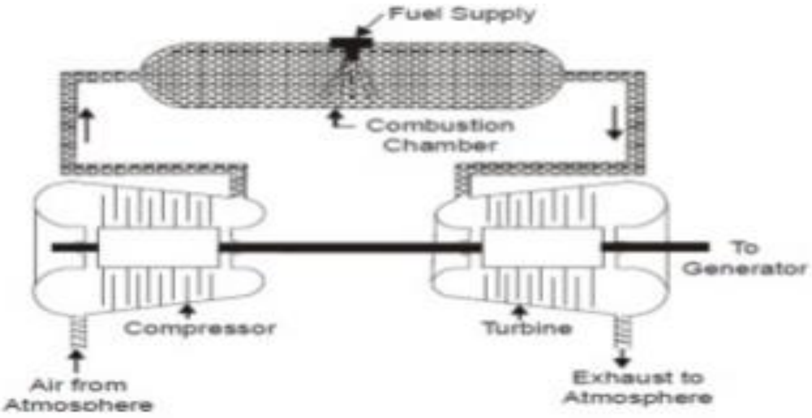
The effect of preheating the fuel and/or oxidizer can be included. An ideal theoretical flame temperature T is computed using energy conservation assuming complete combustion, no dissociation of combustion products, and no heat losses. The energy in the constituents supplied to the combustion process, plus the energy of combustion, is equated to the energy of the combustion products to give,

$$T - T_{ref} = \frac{(\text{energy in feed air and fuel above } T_{ref}) + (\text{energy released by combustion})}{(\text{total mass of products}) \times (\text{mean heat capacity of products})}$$

UNIT III

COMBUSTION IN GAS TURBINE ENGINES

The simplest form of gas turbine requires three components: the gas turbine itself, a compressor, and a combustor in which fuel is mixed with air and burned. These three basic elements are depicted schematically in Figure



Open cycle gas turbine.

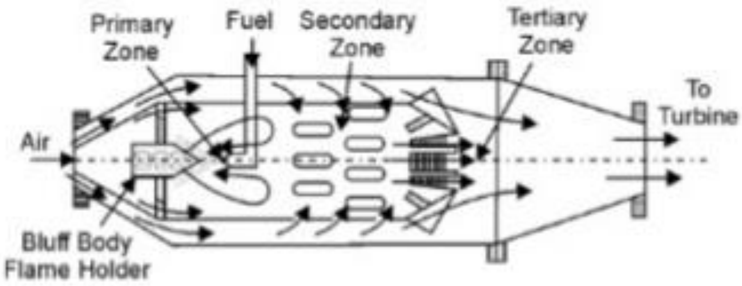
COMBUSTION CHAMBERS

The gas turbine is a continuous flow system; therefore, the combustion in the gas turbine differs from the combustion in diesel engines. High rate of mass flow results in high velocities at various points throughout the cycle (300 m/sec). One of the vital problems associated with the design of gas turbine combustion system is to secure a steady and stable flame inside the combustion chamber. The gas turbine combustion system has to function under certain different operating conditions which are not usually met with the combustion systems of diesel engines. A few of them are listed below:

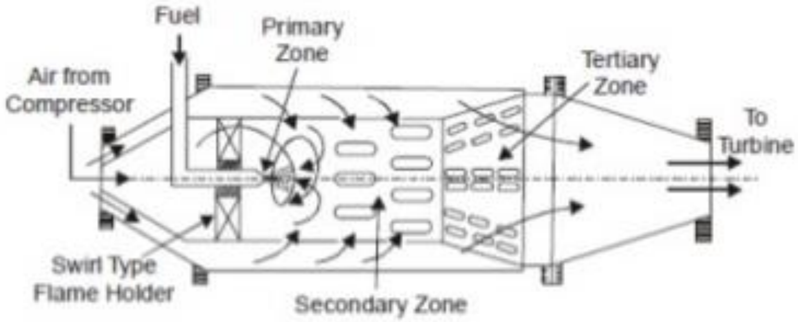
- ✓ Combustion in the gas turbine takes place in a continuous flow system and, therefore, the advantage of high pressure and restricted volume available in diesel engine is lost. The chemical reaction takes place relatively slowly thus requiring large residence time in the combustion chamber in order to achieve complete combustion.

✓ The gas turbine requires about 100:1 air-fuel ratio by weight for the reasons mentioned earlier. But the air-fuel ratio required for the combustion in diesel engine is approximately 15:1. Therefore, it is impossible to ignite and maintain a continuous combustion with such weak mixture. It is necessary to provide rich mixture fm ignition and continuous combustion, and therefore, it is necessary to allow required air in the combustion zone and the remaining air must be added after complete combustion to reduce the gas temperature before passing into the turbine.

✓ A stable continuous flame can be maintained inside the combustion chamber when the stream velocity and fuel burning velocity are equal. Unfortunately most of the fuels have low burning velocities of the order of a few meters per second; therefore, flame stabilization is not possible unless some technique is employed to anchor the flame in the combustion chamber



Combustion Chamber with Upstream Injection with Bluff-body Flame Holder.



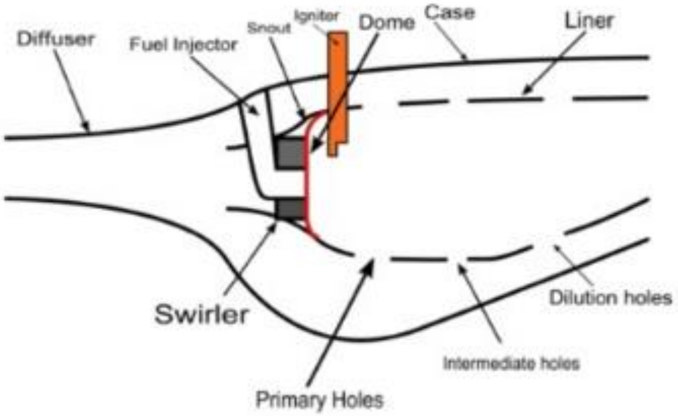
Combustion Chamber with Downstream Injection and Swirl Holder

The common methods of flame stabilization used in practice are bluff body method and swirl flow method. Two types of combustion chambers using bluff body and swirl for flame stabilization. The major difference between two is the use of different methods to create pilot zone for flame stabilization. Nearly 15 t 20% of the total air is passed around the jet of fuel providing rich mixture in the primary zone. This mixture burns continuously in the primary (pilot) zone and produces high temperature gases. About 30% of the total air is supplied in the secondary zone through the annuals around the flame tube to complete the combustion. The secondary air must be admitted at right points in the combustion chamber otherwise the cold injected air may chill the flame locally thereby reducing the rate of reaction. The secondary air helps to complete the combustion as well as helps to cool the flame tube. The remaining 50% air is mixed with burnt gases in the "tertiary zone" to cool the gases down to the Temperature suited to the turbine blade materials. By inserting a bluff body in mainstream, a low-pressure zone is created downstream side that causes the reversal of flow along the axis of the combustion chamber to stabilize the flame. In case of swirl stabilization, the primary air is passed through the swirled, which produces a vortex motion creating a low-pressure zone along the axis of the chamber to cause the reversal of flow. Sufficient turbulence must be created in all three zones of combustion and uniform mixing of hot and cold bases to give uniform temperature gas stream at the outlet of the combustion chamber.

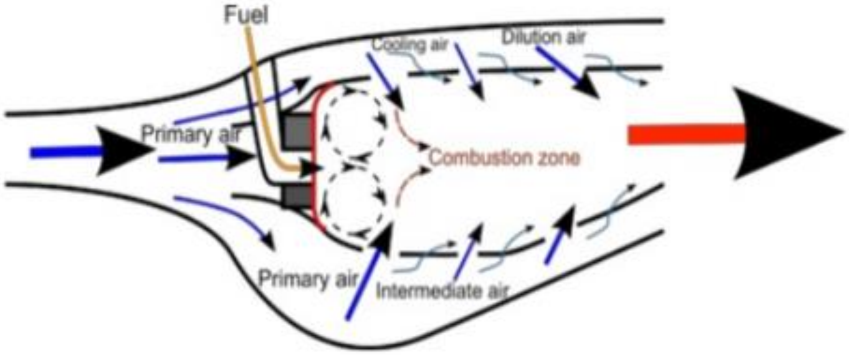
Four steps of Combustion process

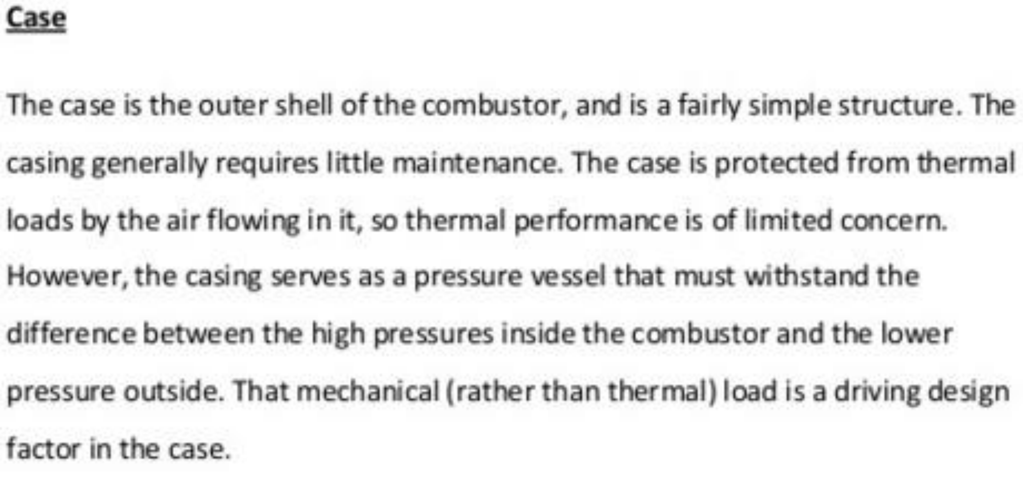
- ⇨ Formulation of reactive mixture
- ⇨ Ignition
- ⇨ Flame propagation
- ⇨ Cooling of combustion product with air

Components



Air flow paths

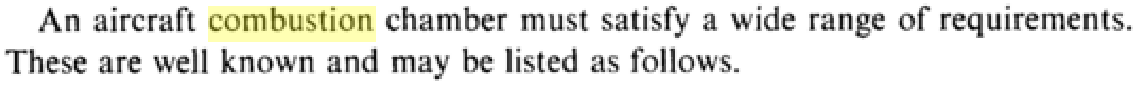




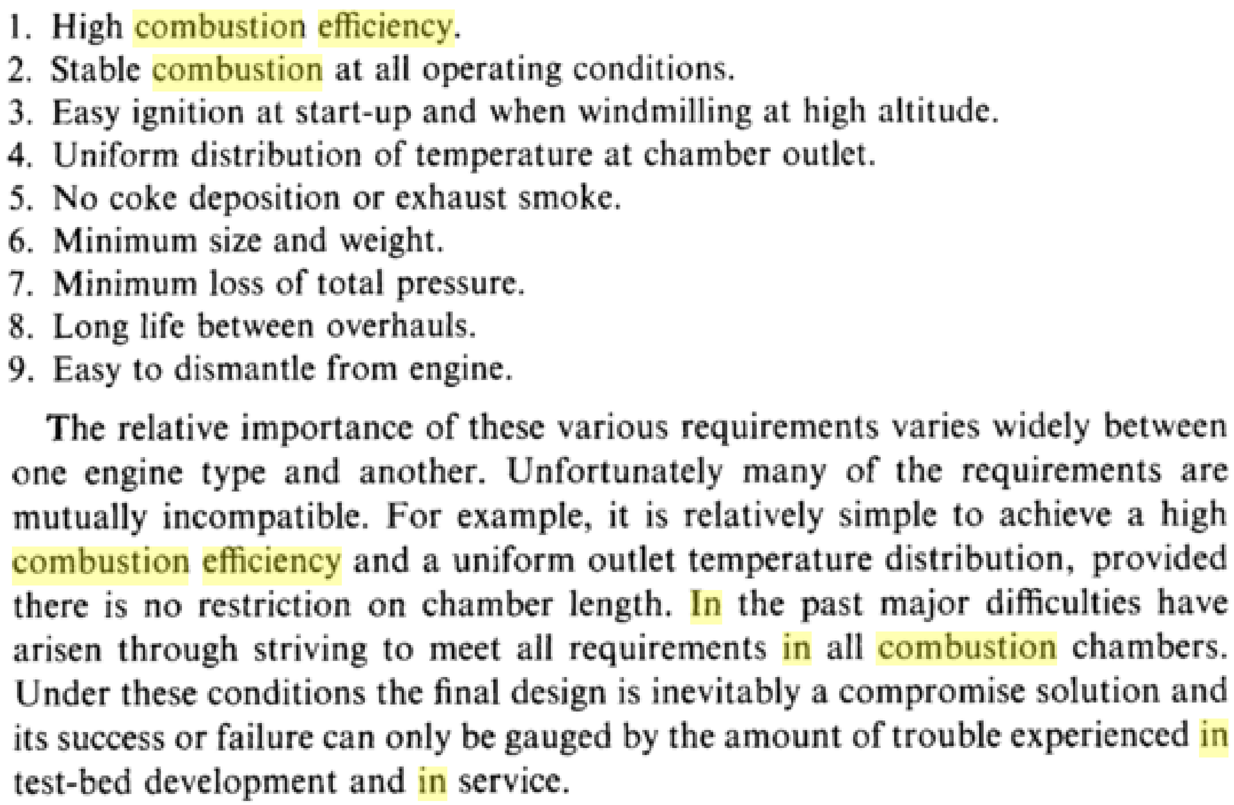
Case

The case is the outer shell of the combustor, and is a fairly simple structure. The casing generally requires little maintenance. The case is protected from thermal loads by the air flowing in it, so thermal performance is of limited concern. However, the casing serves as a pressure vessel that must withstand the difference between the high pressures inside the combustor and the lower pressure outside. That mechanical (rather than thermal) load is a driving design factor in the case.

Performance Requirements



An aircraft combustion chamber must satisfy a wide range of requirements. These are well known and may be listed as follows.

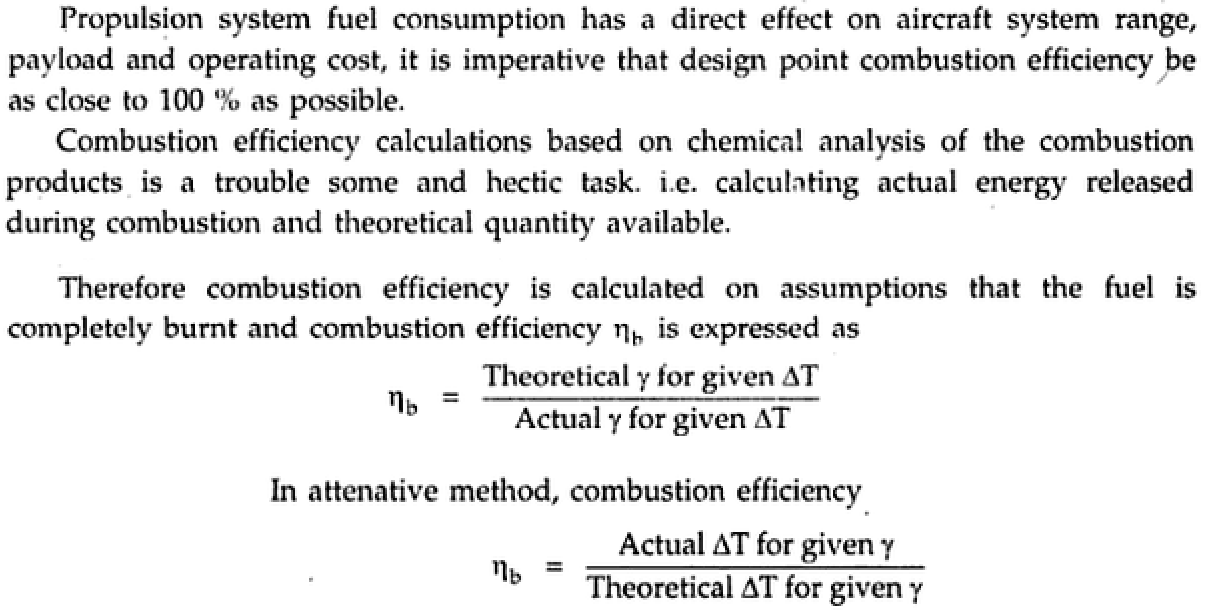


1. High combustion efficiency.
2. Stable combustion at all operating conditions.
3. Easy ignition at start-up and when windmilling at high altitude.
4. Uniform distribution of temperature at chamber outlet.
5. No coke deposition or exhaust smoke.
6. Minimum size and weight.
7. Minimum loss of total pressure.
8. Long life between overhauls.
9. Easy to dismantle from engine.

The relative importance of these various requirements varies widely between one engine type and another. Unfortunately many of the requirements are mutually incompatible. For example, it is relatively simple to achieve a high combustion efficiency and a uniform outlet temperature distribution, provided there is no restriction on chamber length. In the past major difficulties have arisen through striving to meet all requirements in all combustion chambers. Under these conditions the final design is inevitably a compromise solution and its success or failure can only be gauged by the amount of trouble experienced in test-bed development and in service.

COMBUSTION EFFICIENCY

The combustion efficiency of a gas turbine combustion chamber is usually defined as the ratio of the heat actually liberated at the chamber outlet to the heat that would be liberated in an ideal system**.**



Propulsion system fuel consumption has a direct effect on aircraft system range, payload and operating cost, it is imperative that design point combustion efficiency be as close to 100 % as possible.

Combustion efficiency calculations based on chemical analysis of the combustion products is a trouble some and hectic task. i.e. calculating actual energy released during combustion and theoretical quantity available.

Therefore combustion efficiency is calculated on assumptions that the fuel is completely burnt and combustion efficiency η_b is expressed as

$$\eta_b = \frac{\text{Theoretical } \gamma \text{ for given } \Delta T}{\text{Actual } \gamma \text{ for given } \Delta T}$$

In attenative method, combustion efficiency

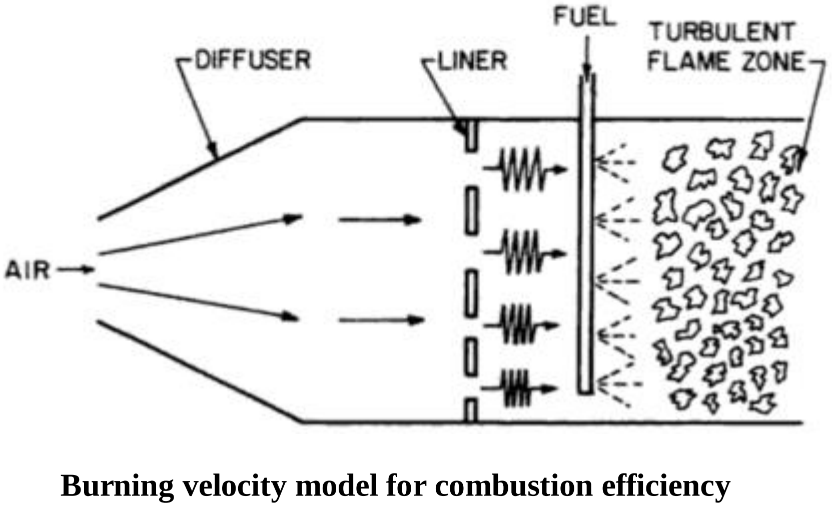
$$\eta_b = \frac{\text{Actual } \Delta T \text{ for given } \gamma}{\text{Theoretical } \Delta T \text{ for given } \gamma}$$

The Combustion Process

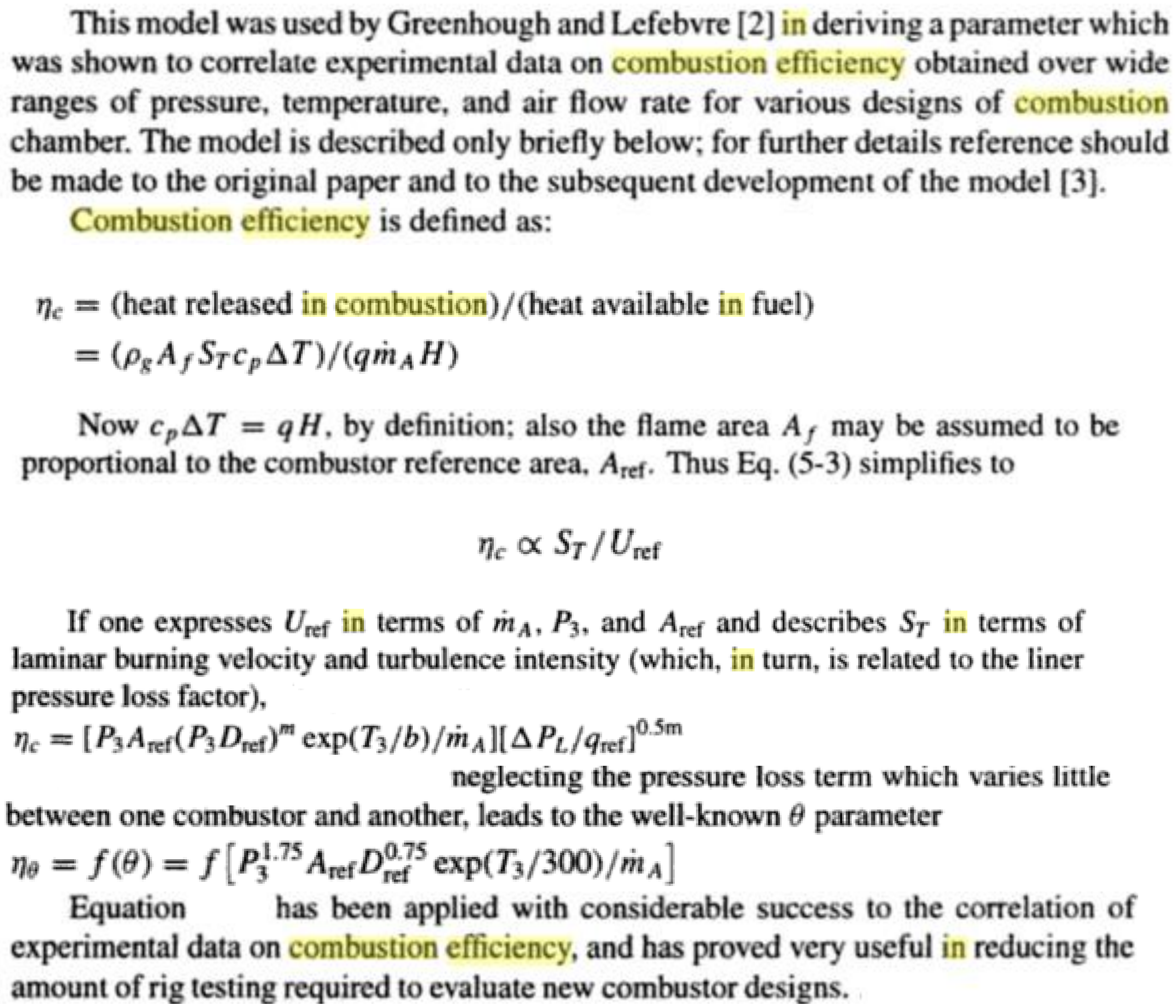
The primary purpose of combustion is to raise the temperature of the airflow by efficient burning of the fuel. From a design viewpoint, an important requirement is a means of relating combustion efficiency to the operating variables of air pressure, temperature, and mass flow rate, and to the combustor dimensions. Unfortunately, the various processes taking place within the combustion zone are highly complex and a detailed theoretical treatment is precluded at this time. Until more information is available, suitable parameters for relating combustion performance to combustor dimensions and operating conditions can be derived only through the use of very simplified models to represent the combustion process. One such model starts from the well-established and widely accepted notion that the total time required to burn a liquid fuel is the sum of the times required for fuel evaporation, mixing of fuel vapor with air and combustion products, and chemical reaction. Because the time available for combustion is inversely proportional to the airflow rate, the combustion efficiency may be expressed [1] as

$$\eta_c = f(\text{airflow rate})^{-1}\left(\frac{1}{\text{evaporation rate}}+\frac{1}{\text{mixing rate}}+\frac{1}{\text{reaction rate}}\right)^{-1}$$

In practical combustion systems, the maximum rate of heat release under any given operating conditions may be governed by either evaporation, mixing, or chemical reaction, but rarely by all three at the same time. However, when the combustion process is in transition from one regime to another, two of the three key rates will participate in determining the overall combustion efficiency. Before exploring that situation, let us examine the separate effects on combustion efficiency of chemical reaction, mixing, and evaporation.



Burning velocity model for combustion efficiency



This model was used by Greenhough and Lefebvre [2] in deriving a parameter which was shown to correlate experimental data on combustion efficiency obtained over wide ranges of pressure, temperature, and air flow rate for various designs of combustion chamber. The model is described only briefly below; for further details reference should be made to the original paper and to the subsequent development of the model [3].

Combustion efficiency is defined as:

$$\eta_c = (\text{heat released in combustion})/(\text{heat available in fuel})$$
$$= (\rho_g A_f S_T c_p \Delta T)/(q \dot{m}_A H)$$

Now $c_p \Delta T = qH$, by definition; also the flame area A_f may be assumed to be proportional to the combustor reference area, A_{ref}. Thus Eq. (5-3) simplifies to

$$\eta_c \propto S_T / U_{\text{ref}}$$

If one expresses U_{ref} in terms of $\dot{m}_A$, P_3, and A_{ref} and describes S_T in terms of laminar burning velocity and turbulence intensity (which, in turn, is related to the liner pressure loss factor),

$$\eta_c = [P_3 A_{\text{ref}} (P_3 D_{\text{ref}})^m \exp(T_3/b)/\dot{m}_A][\Delta P_L/q_{\text{ref}}]^{0.5m}$$

neglecting the pressure loss term which varies little between one combustor and another, leads to the well-known θ parameter

$$\eta_\theta = f(\theta) = f\left[P_3^{1.75} A_{\text{ref}} D_{\text{ref}}^{0.75} \exp(T_3/300)/\dot{m}_A\right]$$

Equation has been applied with considerable success to the correlation of experimental data on combustion efficiency, and has proved very useful in reducing the amount of rig testing required to evaluate new combustor designs.

Factors affecting combustion efficiency:

Gas turbine site performance is directly affected by inlet air density and air environmental conditions. The effects of inlet air density on produced power and heat rate are:

- A given engine design limits air volume flow capacity
- Produced power is a function of actual energy extracted per pound of vapor and mass flow of vapor
- For a given engine therefore, produced power varies directly with inlet air density
- Produced power does become limited by low volume (stall and surge) flow

Care must be taken when selecting gas turbines to ensure sufficient shaft power is available at high temperature conditions and fouled inlet conditions, and gas turbine applications tend to be ‘fully loaded’ since gas turbines (unlike steam turbines) are not custom designed.

Thermal efficiency is a prime factor in gas turbine performance. It is the ratio of net work produced by the engine to the chemical energy supplied in the form of fuel. The three most important factors affecting the thermal efficiency are turbine inlet temperature, compression ratio, and the component efficiencies of the compressor and turbine. Other factors that affect thermal efficiency are compressor inlet temperature and combustion efficiency.

The effects that compressor and turbine component efficiencies have on thermal efficiency when turbine and compressor inlet temperatures remain constant are shown in Figure 1. In actual operation, the turbine engine exhaust temperature varies directly with turbine inlet temperature at a constant compression ratio.

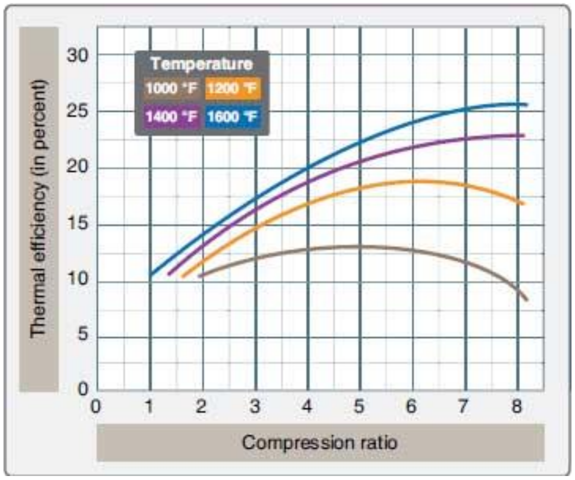


Fig.1. *The effect of compression ratio on thermal efficiency.*

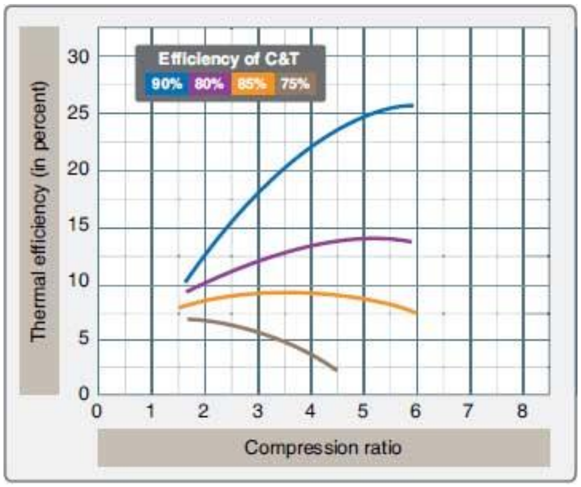


Fig. 2. Turbine and compressor efficiency vs. thermal efficiency.

maximum thermal efficiency can be obtained by maintaining the highest possible exhaust temperature. Since engine life is greatly reduced at high turbine inlet temperatures, the operator should not exceed the exhaust temperatures specified for continuous operation. Figure 2 illustrates the effect of turbine inlet temperature on turbine blade life. In the previous discussion, it was assumed that the state of the air at the inlet to the compressor remains constant.

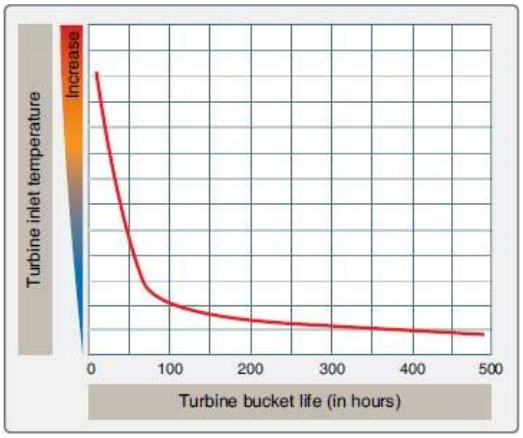


Fig.3. *Effect of turbine inlet temperature on turbine bucket life.*

The power produced by a turbine engine is proportional to the stagnation density at the inlet. The next three illustrations show how changing the density by varying altitude, airspeed, and outside air temperature affects the power level of the engine. Figure.4 shows that the thrust output improves rapidly with a reduction in outside air temperature (OAT) at constant altitude, rpm, and airspeed. This increase occurs partly because the energy required per pound of airflow to drive the compressor varies directly with the temperature, leaving more energy to develop thrust. In addition, the thrust output increases since the air at reduced temperature has an increased density. The increase in density causes the mass flow through the engine to increase. The altitude effect on thrust, as shown in Figure 5, can also be discussed as a density and temperature effect. In this case, an increase in altitude causes a decrease in pressure and temperature.

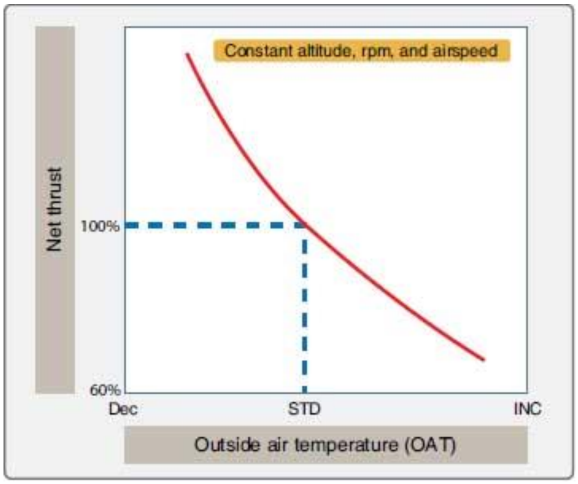


fig.4. *Effect of OAT on thrust output.*

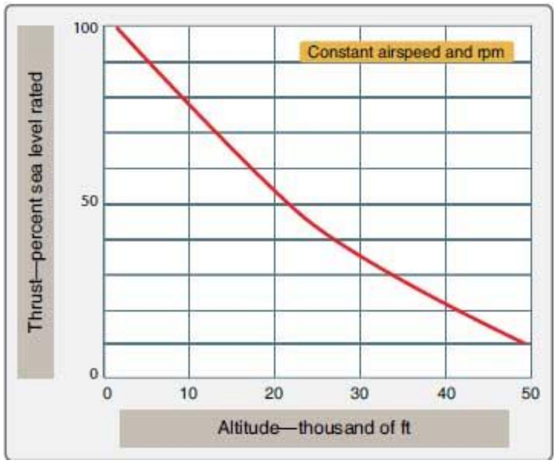
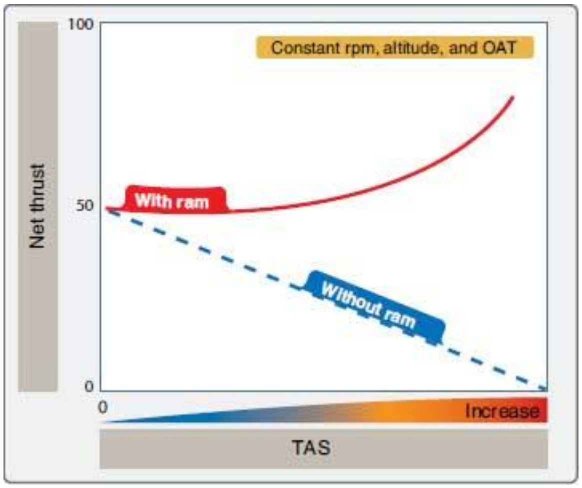


fig. 5.Effect of altitude on thrust output.

The effect of airspeed on the thrust of a gas-turbine engine is shown in Figure 6. To explain the airspeed effect, it is necessary to understand first the effect of airspeed on the factors that combine to produce net thrust: specific thrust and engine airflow. Specific thrust is the net thrust in pounds developed per pound of airflow per second. It is the remainder of specific gross thrust minus specific ram drag. As airspeed is increased, ram drag increases rapidly. The exhaust velocity remains relatively constant; thus, the effect of the increase in airspeed results in decreased specific thrust. [Figure 7] In the low-speed range, the specific thrust decreases faster than the airflow increases and causes a decrease in net thrust. As the airspeed increases into the higher range, the airflow increases faster than the specific thrust decreases and causes the net thrust to increase until sonic velocity is reached. The effect of the combination on net thrust is illustrated in Figure 7.



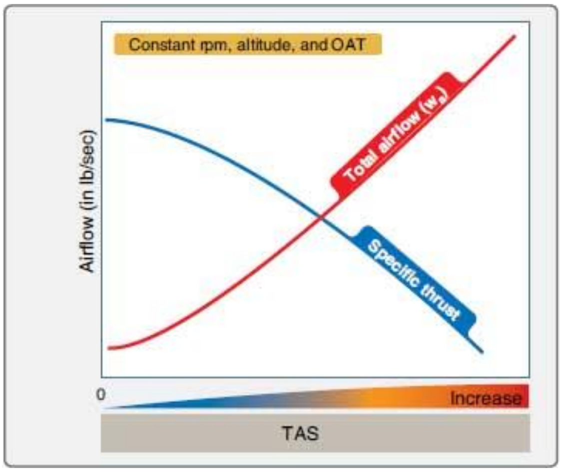


Fig. 6 Effect of airspeed on net thrust.

Fig.7. Effect of airspeed on specific thrust and total engine airflow.

FUELS USED FOR GAS TURBINE COMBUSTION CHAMBERS

The gas turbine's major advantage has been its inherent fuel flexibility. Fuel candidates encompass the entire spectrum from gases to solids. Gaseous fuels traditionally include natural gas, process gas, low-Btu coal gas, and vaporized fuel oil gas. "Process gas" is a broad term used to describe gas formed by some industrial process. Process gases include refinery gas, producer gas, coke oven gas, and blast furnace gas among others. Natural gas is the fuel of choice and is usually the basis on which performance for a gas turbine is compared, since it is a clean fuel fostering longer machine life.

Vaporized fuel oil gas behaves very closely to natural gas because it provides high performance with a minimum reduction of component life. About 40% of the turbine power installed operates on liquid fuels. Liquid fuels can vary from light volatile naphtha through kerosene to the heavy viscous residuals.

Table 12-1
Comparison of Liquid Fuels for Gas Turbines

General Fuel Type	True Distillate & Naphthas	Blended Heavy Distillates & Low-Ash Crudes	Residuals & High-Ash Crude
Fuel pre-heat	No	Yes	Yes
Fuel atomization	Mech/LP air	HP/LP air	HP air
Desalting	No	Some	Yes
Fuel inhibitation	Usually none	Limited	Always
Turbine washing	No	Yes, except distillate	Yes
Start-up fuel	With naphtha	Some fuels	Always
Base fuel cost	Highest	Intermediate	Lowest
Description	High-quality distillate essentially ash-free	Low-ash, limited contaminant levels	Low-volatility High-ash
Types of fuels included	True distillates (naphtha, kerosene, no. 2 diesel, no. 2 fuel oil, JP-4, JP-5)	High-quality crudes, slightly contaminated distillates Navy distillate	Residuals and low-grade crude (No. 5 fuel, No. 6 fuel, Bunker C)
ASTM designation	1-GT, 2-GT, 3-GT	3-GT	4-GT
Turbine inlet temperature	Highest	Intermediate	Lowest

Fuel Specifications

The following are some fuel requirements that are important in designing a combustion system and any necessary fuel treatment equipment:

1. Heating value
2. Cleanliness
3. Corrosivity
4. Deposition and fouling tendencies
5. Availability

The heating of a fuel affects the overall size of the fuel system. Generally, fuel heating is a more important concern in connection with gaseous fuels, since liquid fuels all come from petroleum crude and show narrow heating-value variations. Gaseous fuels, on the other hand, can vary from 1100 Btu/ft^3 (41,000 KJ/m^3) for natural gas to (11,184 KJ/m^3) or below for process gas. The fuel system will of necessity have to be larger for the process gas, since more is required for the same temperature rise.

Cleanliness of the fuel must be monitored if the fuel is naturally "dirty" or can pick up contaminants during transportation. The nature of the contaminants depends on the particular fuel. The definition of cleanliness here concerns particulates that can be strained out and is not concerned with soluble contaminants. These contaminants can cause damage or fouling in the fuel system and result in poor combustion.

Corrosion by the fuel usually occurs in the hot section of the engine, either in the combustor or the turbine blading. Corrosion is related to the amounts of certain heavy metals in the fuel. Fuel corrosivity can be greatly reduced by specific treatments discussed later in this chapter.

Deposition and fouling can occur in the fuel system and in the hot section of the turbine. Deposition rates depend on the amounts of certain compounds contained in the fuel. Some compounds that cause deposits can be removed by fuel treating.

Finally, fuel availability must be considered. If future reserves are unknown, or seasonal variations are expected, dual fuel capability must be considered.

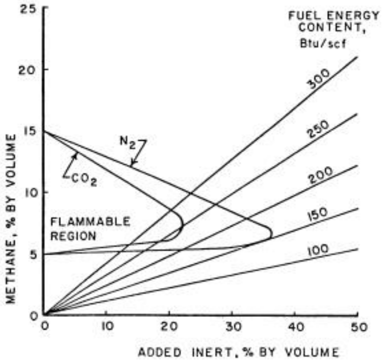
Gaseous Fuel Specifications

Heating value	300–1100 Btu/ft^3 (11,184–41,000 KJ/m^3)
Solid contaminants	< 30ppm
Flammability limits	2.2:1
Composition—S, Na, K, Li	< 5ppm
(Sulfur + sodium + potassium + lithium)	(When formed into alkali metasulfate)
H_2O (by weight)	< 25%

Natural gas has a Btu content of about 1000–1100 Btu/ft^3 (37,272–41,000 KJ/m^3). By definition, low-Btu gases can vary between 100–350 Btu/ft^3 (3728–13,048 KJ/m^3). Presently, little success has been achieved in burning gases with a heating value lower than 200 Btu/ft^3 (7456 KJ/m^3). To provide the same energy as natural gas, a 150 Btu/ft^3 (5592 KJ/m^3) low-Btu gas must be utilized at the rate of seven times that of natural gas on a volumetric basis.

Therefore, the mass flow rate to provide the same energy must be about 8–10 times that of natural gas. The flammability of low-Btu gases is very much dependent on the mixture of CH_4 and other inert gases. Figure 12-2 shows this effect by illustrating that a mixture of CH_4-CO_2 of less than 240 Btu/ft^3 (8947 KJ/m^3) is inflammable, and a CH_4-N_2 mixture of less than about 150 Btu/ft^3 is less inflammable.

Low-Btu gases near these values have greatly restricted flammability limits when compared to CH_4 in the air. Vaporized fuel oil gas is produced by mixing superheated steam with oil and then vaporizing the oil to provide a gas whose properties and heating value are close to natural gas.



Flammable fuel mixtures of CH_4-N_2 and CH_4-CO_2 at one atm showing various energy levels.

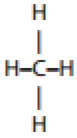
Alternative Fuels

Types of Hydrocarbons

Pure hydrocarbon fuels are compounds of two elements only, carbon and hydrogen. They may be gaseous, liquid, or solid at normal pressure and temperature, depending on the number of carbon atoms and their molecular structure. Those with up to four carbon atoms are gaseous; those with twenty or more are solid, and those in between are liquid. It is usual to classify the hydrocarbons present in petroleum fuel into four main groups: paraffinic, olefinic, naphthenic, and aromatic. The proportions in which these groups are present largely define the character of the fuel.

Paraffins:

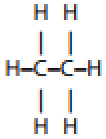
Paraffinic oils are found mainly in the United States, North Africa, and Nigeria. They have the general formula C_nH_{2n+2}. Thus, the simplest hydrocarbon, methane, is in this class; its molecule can be represented as:



$$\begin{array}{c}H\\|\\H-C-H\\|\\H\end{array}$$

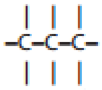
Methane, CH_4

The remaining normal paraffins are built up from methane as straight chains, e.g.



$$\begin{array}{c}H\;\;H\\|\;\;|\\H-C-C-H\\|\;\;|\\H\;\;H\end{array}$$

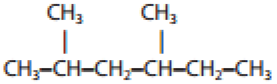
Ethane, C_2H_6



$$\begin{array}{c}|\;\;|\;\;|\\-C-C-C-\\|\;\;|\;\;|\end{array}$$

Propane, C_3H_8

Alternative paraffin configurations, or isoparaffins, are in the form of branched chains, such as



$$CH_3-\overset{\overset{CH_3}{|}}{CH}-CH_2-\overset{\overset{CH_3}{|}}{CH}-CH_2-CH_3$$

Dimethyl hexane, $C_6H_{12}(CH_3)_2$

Current aviation fuels contain an average of 60% paraffins, depending on the source of the crude oil and the distillation process. In general, paraffins tend to have a higher hydrogen/carbon ratio, lower density, lower freeze point, and high gravimetric calorific value than other types of hydrocarbon fuels.

Olefins

Olefins conform to the general formula C_nH_{2n}. They do not normally exist in crude oil, but are produced by conversion processes in the refinery. As olefins are unsaturated, i.e., their molecules contain less than the maximum possible number of hydrogen atoms, they are very active chemically and readily react with a great many compounds to form resinous gums and rubberlike materials.

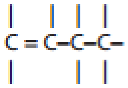
Olefin molecules must contain at least two carbon molecules, and the lightest molecule is, therefore, C_2H_4, ethylene. More complex molecules of the olefin series are obtained by adding CH_2, as in

$$\begin{array}{c}|\;\;|\\C=C\\|\;\;|\end{array}$$

Ethylene, C_2H_4

$$\begin{array}{l}|\;\;|\;\;\;|\\C=C-C-\\|\;\;\;\;\;\;|\end{array}$$

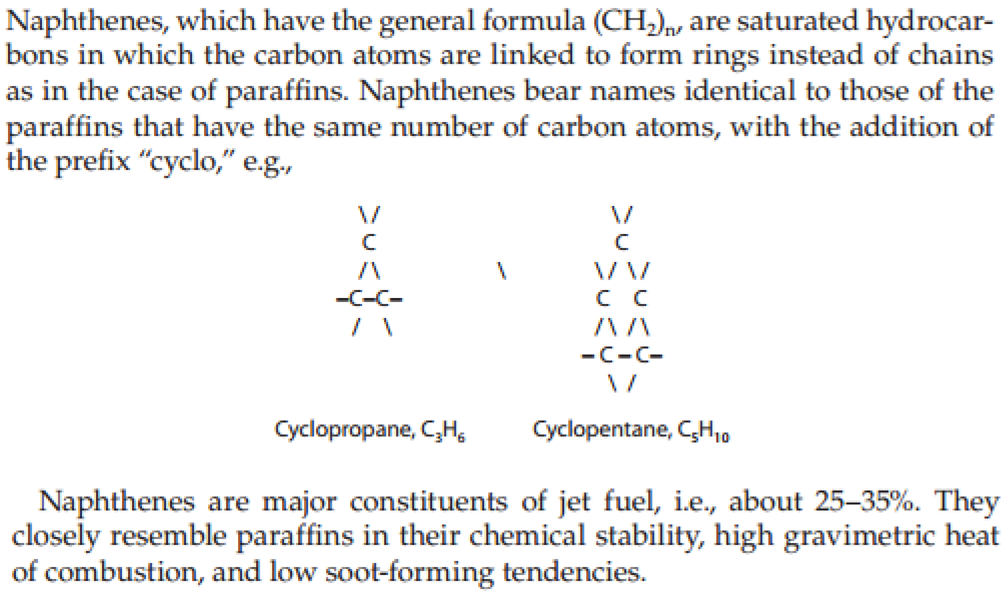
Propylene, C_3H_6



$$\begin{array}{l}|\;\;\;\;|\;\;|\;\;|\\C=C-C-C-\\|\;\;\;\;\;\;\;|\;\;|\end{array}$$

Butylene, C_4H_8

Naphthenes



Naphthenes, which have the general formula $(CH_2)_n$, are saturated hydrocarbons in which the carbon atoms are linked to form rings instead of chains as in the case of paraffins. Naphthenes bear names identical to those of the paraffins that have the same number of carbon atoms, with the addition of the prefix "cyclo," e.g.,

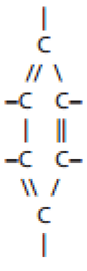
Cyclopropane, C_3H_6 Cyclopentane, C_5H_{10}

Naphthenes are major constituents of jet fuel, i.e., about 25–35%. They closely resemble paraffins in their chemical stability, high gravimetric heat of combustion, and low soot-forming tendencies.

Aromatics

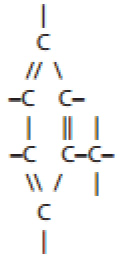
Aromatics are ring compounds containing one or more six-member rings with the equivalent of three double bonds. Although similar in structure to the naphthenes, they contain less hydrogen and, in consequence, their specific energy is appreciably lower. Aromatic compounds in fuel cause swelling of o-ring and this helps seal the high pressure aircraft fuel system. The disadvantages of aromatic compounds include a marked tendency to soot formation and a high hygroscopicity that can lead to precipitation of ice crystals when the fuel is subjected to low temperatures. Aromatics also have a strong solvent action on rubber that can cause trouble in fuel systems and on aircraft fitted with soft-rubber-lined fuel tanks.

The characteristic formula for the aromatics is C_nH_{2n-6}. The simplest member is benzene, in which each carbon atom carries only one hydrogen atom:



Benzene, C_6H_6

More complex molecules of the aromatic group are obtained either by replacing one or more of the hydrogen atoms with hydrocarbon groups or by "condensing" one or more rings [8]. Another example is:



Toluene, $C_6H_5CH_3$

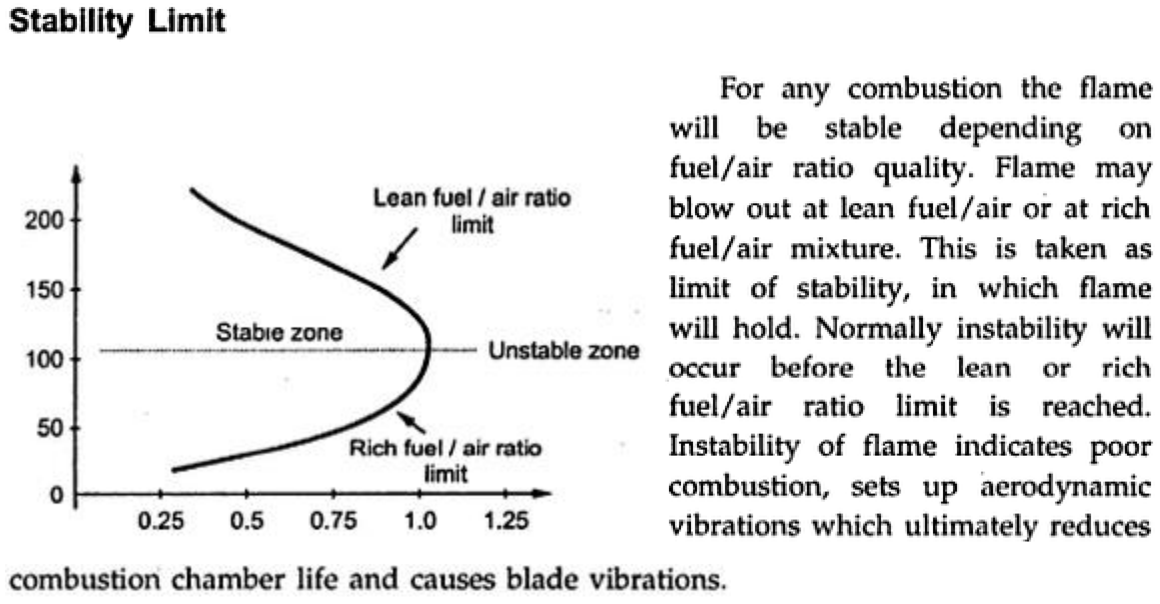
Production of Liquid Fuels

1. **Separation process**: Crude oil is separated into its primary fractions, consisting of gasoline, distillate fuels, and fuel oil; these then provide the basic material for the desired range of fuel products. Separation is accomplished by a distillation process that exploits the fact that the various components in crude oil have different boiling points. When a crude oil is heated, the first gases evolved are chiefly methane, ethane, propane, and butane. Next, vapors are released that condense to form light distillates and then gasoline. As boiling proceeds, kerosine emerges, followed by the middle distillates used in gas oil and diesel fuel. Finally, a residue is left that is used in the manufacture of lubricating oils, wax, and bitumen.

2. **Upgrading process**: These processes improve the quality by using chemical reactions to remove any compounds present in trace quantities. Commonly used upgrading processes are sweetening, hydrotreating, and clay treatment.

3. **Conversion process**: These processes change the molecular structure of the feedstock, usually by "cracking" large molecules into small ones, e.g., catalytic cracking and hydrocracking.

COMBUSTION STABILITY:



Stability Limit

For any combustion the flame will be stable depending on fuel/air ratio quality. Flame may blow out at lean fuel/air or at rich fuel/air mixture. This is taken as limit of stability, in which flame will hold. Normally instability will occur before the lean or rich fuel/air ratio limit is reached. Instability of flame indicates poor combustion, sets up aerodynamic vibrations which ultimately reduces combustion chamber life and causes blade vibrations.

Combustion stability → The ability of the combustion process to sustain itself in a continuous manner.

Combustion stability depends on mass flow rate, combustion volume and pressure along with fuel/air ratio. All these are combined into the Combustor Loading Parameter (CLP) which is defined as

$$CLP = \frac{\dot{m}}{P^n \text{(combustion volume)}}$$

n = no of molecules in fuel
= 1.8 when hydrocarbon is burned in air
= 1 under high-pressure conditions.

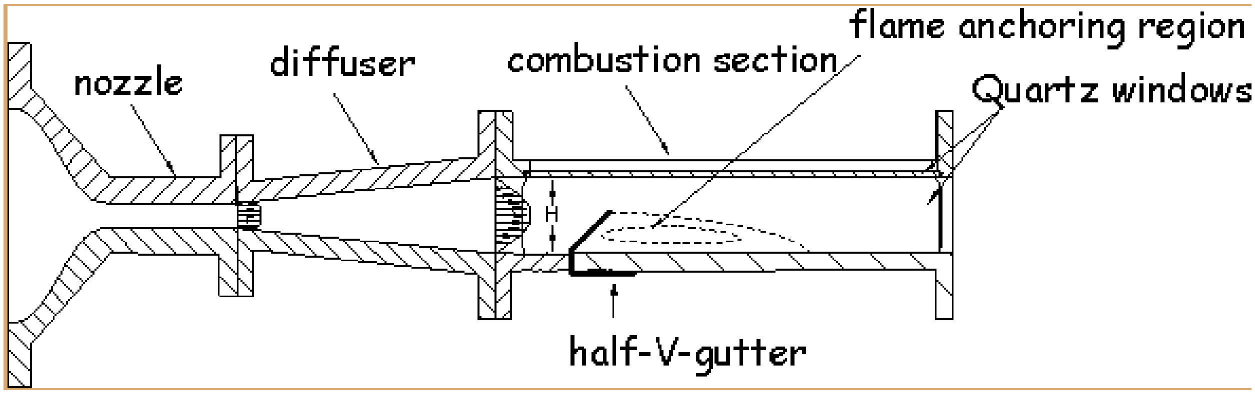
To have a stable flame, the velocity of the mixture must be maintained within certain limits. If the velocity is too high, the flame will be blown out the exit and if the velocity is too low, the flame will travel upstream and be extinguished. Normally the combustion chambers are designed with an inlet air velocity not exceeding 80 m/s at design load.

FLAME HOLDER

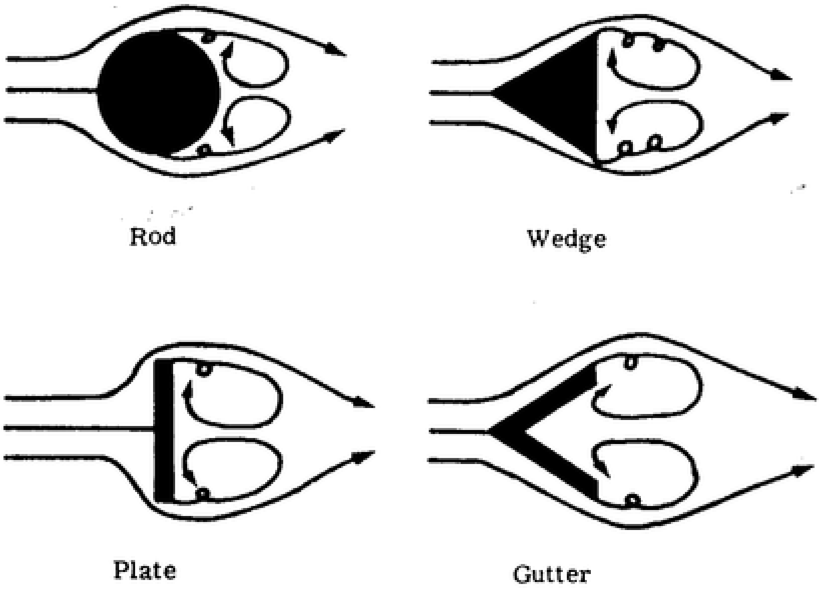
A flame holder is a component of a jet engine designed to help maintain continual combustion.All continuous-combustion jet engines require a flame holder. A flame holder creates a low-speed eddy in the engine to prevent the flame from being blown out. The design of the flame holder is an issue of balance between a stable eddy and drag.

The simplest design, often used in amateur projects, is the can-type flame holder, which consists of a can covered in small holes. Much more effective is the H-gutter flame holder, which is shaped like a letter H with a curve facing and opposing the flow of air. Even more effective, however, is the V-gutter flame holder, which is shaped like a V with the point in the direction facing the flow of air. Some studies have suggested that adding a small amount of base bleed to a V-gutter helps reduce drag without reducing effectiveness. In fluid dynamics, an **eddy** is the swirling of a fluid and the reverse current created when the fluid flows past an obstacle. The moving fluid creates a space devoid of downstream-flowing fluid on the downstream side of the object.

Fluid behind the obstacle flows into the void creating a swirl of fluid on each edge of the obstacle, followed by a short reverse flow of fluid behind the obstacle flowing upstream, toward the back of the obstacle. This phenomenon is most visible behind large emergent rocks in swiftflowing rivers.



Re-circulation in flames

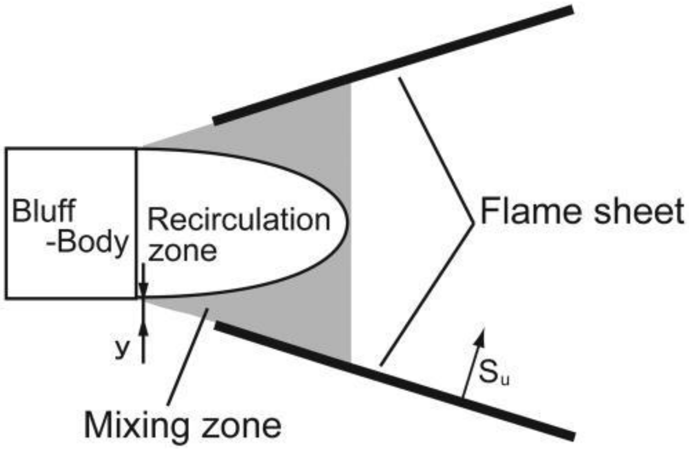

Rod

Wedge

Plate

Gutter

Figure 8.31 Flame stabilization by recirculation



UNIT IV

COMBUSTION IN ROCKETS

Basic Rocket propulsion:

To launch a rocket or to move a rocket through space, we must use a propulsion system to generate thrust. For rocket propulsion the fuel and oxidizer are usually stored as either a liquid or a solid. During combustion, new chemical substances are created from the fuel and the oxidizer.

SOLID PROPELLANTS

Solid propellants are classified into the following four categories:

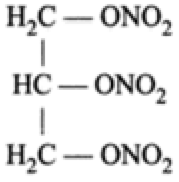
(a) Double-base or homogeneous propellants,
(b) Composite or heterogeneous propellants,
(c) Composite modified double-base propellants, and
(d) Nitramine propellants.

The composition and salient features of these propellants are discussed in the following sections.

Double-base Propellants

The propellants comprise nitrocellulose (NC) and nitroglycerine (NG) mixed together at the molecular level to form a homogeneous substance. NC constitutes the fuel. Part of the hydroxyl radicals (OH) in cellulose, which consists of carbon, hydrogen and oxygen in a linear structure $[C_6H_{10}O_5]_n$ is substituted by the nitrate radical ONO_2 in NC to give a molecular structure $[C_6H_{10-x}O_{5-x}(NO_3)_x]_n$. The part of hydroxyl radicals, replaced by ONO_2, is represented by '*x*' in the above molecular formula and would vary depending on the amount of nitration.

NG, whose chemical formula is $[C_3H_5(ONO_2)_3]$, is based on glycerine or propane triol $[C_3H_5(OH)_3]$. The OH radical of glycerine is replaced by ONO_2 to form NG. NG is oxidiser-rich. The chemical structure of NG is aliphatic with a straight chain structure shown below:



$$\begin{array}{l} H_2C - ONO_2 \\ \;| \\ HC - ONO_2 \\ \;| \\ H_2C - ONO_2 \end{array}$$

Both NC and NG can be used singly as propellants since they have both oxidiser and fuel in them. These are known as single base propellants.

When NC and NG are used together, they constitute double-base propellant. NG forms a colloid when properly compounded with NC in the presence of a few additives comprising a plasticiser, such as, diethyl phthalate and triacetin, and stabiliser, such as, diphenylamine. Plasticisers not only increase the fluidity but also make the propellant less sensitive to ignition from impact.

Composite Propellants

The propellant is heterogeneous with a solid crystalline oxidiser, such as, ammonium perchlorate (NH_4ClO_4) dispersed in a polymeric fuel. Metal aluminium powder is also added to enhance the energy released during combustion. The polymer binds together the discrete crystalline oxidiser particles and the metal powder to form a tough rubbery mass. The polymeric fuel is, therefore, referred to as binder.

(a) Oxidiser

Ammonium Perchlorate (AP) is generally used for the oxidiser. Unlike other solid oxidisers, such as, ammonium nitrate (NH_4NO_3) and potassium nitrate (KNO_3), AP dissociates easily and is not very hygroscopic, and hence is preferred. There are many energetic perchlorate-containing compounds with lower negative heats of formation, such as, nitronium perchlorate (NO_2ClO_4), hydrazinium perchlorate ($N_2H_5ClO_4$), and hydrazinium diperchlorate [$N_2H_6(ClO_4)_2$]. However, they have poorer compatibility with the polymeric binder and have lower thermal stability with the result that processing of the propellant and storage becomes problematic. More energetic oxidisers, such as, hydrazinium nitroformate [$N_2H_5C(NO_2)_3$] are being investigated for high performance composite propellants.

Toxic gases, such as hydrochloric acid formed during combustion of AP and hydrazinium perchlorates with polymeric fuels, pollute the environment. The possibilities of using environmental-friendly energetic oxidiser ammonium dinitramide (ADN) are being studied.

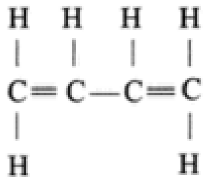
(b) Polymeric Fuel

The polymeric fuel called binder consists of H, C and O atoms (sometimes N and S also). The atomic number of sulphur is 16 compared to 6 for carbon and 1 for hydrogen. Sulphur is, therefore, not a desirable constituent since its atomic mass is high and would result in combustion products with larger molecular mass.

Saturated hydrocarbons (alkanes), in which carbon atoms are attached to each other by means of single bonds, have small but negative values of heats of formation and make good binders. Alkenes with one double bond between carbon atoms, alkadienes with two double bonds, alkynes with one triple bond and alkadiynes with multiple triple bonds between carbon atoms are said to be unsaturated. These have large and negative values of heat of formation.

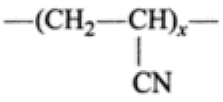
The hydrocarbons could have a straight chain of alkanes, alkenes, alkadienes, alkynes and alkadiynes or could have ring chains in which case they are known as cycloalkanes, cycloalkenes, etc. These straight chain and ring chain hydrocarbons are known as aliphatic compounds and are distinctly different from the aromatic hydrocarbons which have six carbon rings with three double bonds (benzene).

The aliphatic compounds especially those with simpler bond structures are to be preferred as they have smaller negative values of heat of formation. However, most of them like methane, ethane, propane and butane are gases. Polymers with multiple cyclo-butadienes in a linear chain structure are, therefore, chosen. These are called Polybutadienes. The butadiene structure comprising alkadienes with four carbon atoms and two double bonds is shown as follows.



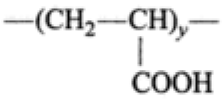
$$\begin{array}{ccccccc} H & & H & & H & & H \\ | & & | & & | & & | \\ C & = & C & - & C & = & C \\ | & & & & & & | \\ H & & & & & & H \end{array}$$

The polybutadiene chain structure is $-(CH_2{=}CH - CH{=}CH_2)_n-$. Here n is the number of butadiene groups. The polybutadiene chain could be attached to poly-acrylo-nitrile group and acrylic acid groups given by:



$$-(\underset{\displaystyle\qquad CN}{CH_2-\overset{}{CH}})_x-$$

Acrylo-nitrile

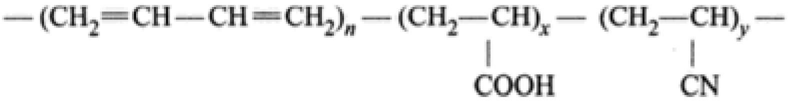


$$-(\underset{\displaystyle\qquad COOH}{CH_2-\overset{}{CH}})_y-$$

Acrylic acid

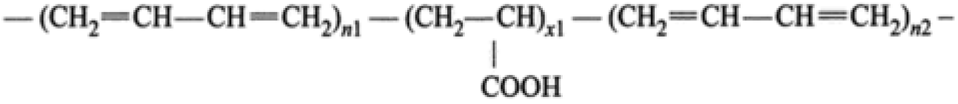
to form polybutadiene acrylic acid acrylonitrile (PBAN).

Carboxy and nitrile groups get attached to the butadiene chain to form a highly cross-linked chain network. The PBAN binder with the linear and cross chains has lower ultimate tensile strength with smaller elongation. It has been used for making propellant grains for large rockets, such as, the solid rocket booster of the Space Shuttle. The structure of the PBAN binder is given below:



$$—(\mathrm{CH_2{=}CH{—}CH{=}CH_2})_n—(\mathrm{CH_2}—\underset{\mathrm{COOH}}{\underset{|}{\mathrm{CH}}})_x—(\mathrm{CH_2}—\underset{\mathrm{CN}}{\underset{|}{\mathrm{CH}}})_y—$$

The randomness of the cross linking can be reduced by removing the carboxyl groups in PBAN and locating them at the ends of the butadiene chain. This provides better mechanical properties to the binder. The binder with the carboxyl radicals located in a controlled way at the ends of the butadiene chain is known as Carboxy Terminated Poly Butadiene (CTPB).



$$—(\mathrm{CH_2{=}CH{—}CH{=}CH_2})_{n1}—(\mathrm{CH_2}—\underset{\mathrm{COOH}}{\underset{|}{\mathrm{CH}}})_{x1}—(\mathrm{CH_2{=}CH{—}CH{=}CH_2})_{n2}-$$

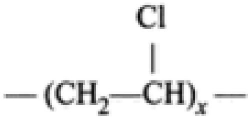
If the carboxyl radical at the chain ends are replaced by hydroxyl (OH) radical, the binder would give higher performance in a propellant. This is because H in the OH radical has a lower atomic number than C in COOH and the energetics of the hydrogen is superior to carbon. The butadiene chains terminated with OH at the ends is called Hydroxy Terminated Poly Butadiene (HTPB). High performance propellants make use of HTPB.

$$\mathrm{HO}—(\mathrm{CH_2{=}CH{—}CH{=}CH_2})_n—\mathrm{OH}$$

HTPB and PBAN binders are most widely used for the manufacture of composite propellants.

The molecular mass of the binders are large considering the long chain, typical values ranging from 30,000 to 1,00,000 kg/kmole.

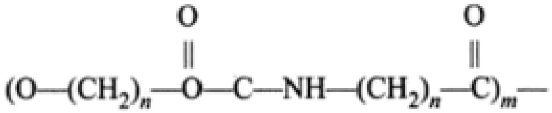
Polyvinyl chloride (PVC) was used earlier as the binder. It consists of the chain:



$$—(\mathrm{CH_2}—\overset{\mathrm{Cl}}{\overset{|}{\mathrm{CH}}})_x—$$

It gives poor performance as it contains less carbon and hydrogen.

Polyurethanes have been used in the past like PVC. They are good energy-wise but contain oxygen and are sensitive to moisture. The chemical structure of polyurethane is given below:



$$(\mathrm{O}—(\mathrm{CH_2})_n—\mathrm{O}—\overset{\mathrm{O}}{\overset{\|}{\mathrm{C}}}—\mathrm{NH}—(\mathrm{CH_2})_n—\overset{\mathrm{O}}{\overset{\|}{\mathrm{C}}})_m—$$

Certain high energy polymers, such as, Glycidyl Azide Polymer (GAP), contain larger percentage of hydrogen and provide higher performance.

Metals:

Metal powders, such as, aluminium are also used as fuel in order to enhance the energy release from combustion since metal combustion is highly exothermic. Aluminium is a light metal and is, therefore, preferable. The aluminium oxide formed as a product of combustion was seen to have a very high negative value of heat of formation (Fig. 4.3).

The use of metal hydrides instead of metals has been thought of with a view to have as much hydrogen in the propellant as possible. The hydrogen, as seen earlier, would contribute to enhancing the specific impulse by lowering the molecular mass of the combustion products. The hydrides are not very compatible with polymeric binders and their use has not been demonstrated in practice.

LIQUID PROPELLANTS

Liquid propellants comprise liquid fuels and liquid oxidisers. They are classified according to their energy content, their ignitability and their storage. In the following, we examine the different liquid propellants based on the above classification.

Energy Content of Propellant

Energy refers to the heat of combustion. It was seen earlier in this chapter that higher energy release is obtained from fuels and oxidisers having small and negative values of heats of formation or positive heats of formation. The fuels considered were kerosene, hydrazine, mono-methyl hydrazine and hydrogen while the oxidisers consisted oxygen, N_2O_4 and HNO_3.

Liquid propellants are categorised as per their specific impulse into:

(a) Low-energy propellants
(b) Medium-energy propellants, and
(c) High-energy propellants.

The classification is said to be based on energy though it is actually done on the basis of specific impulse. The specific impulse takes into account the molecular mass of the combustion products in addition to the energy released by the propellant.

Low-energy Propellants

The low energy propellants are those which give I_{sp} at sea-level conditions less than about 3000 Ns/kg. They comprise liquid oxygen (LO_2) and alcohol which was successfully used in the V2 rockets during the Second World War. Liquid oxygen and kerosene, also known as rocket propellant (RP) and certain combinations of oxidisers and fuels, such as, nitric acid with aniline, xylidine or hydrazine and N_2O_4 with hydrazine, mono-methyl hydrazine and unsymmetrical di-methyl hydrazine also constitute the low energy propellants. The characteristics of these propellants are discussed in the following:

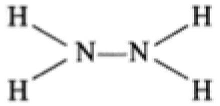
Aniline (C_6H_7N) is an aromatic amine in which the amine radical NH_2 is attached to the benzene chain. In the case of xylidine ($C_8H_{11}N$) two methyl radicals are additionally attached to the benzene chain.

Both aniline and xylidine react spontaneously with nitric acid (HNO_3) when brought in contact in the liquid phase itself. The combustion products, however, contain a lot of soot considering the aromatic nature of the fuel. The energy release is low since the heats of formation of both the fuels (about –100 kJ/mole) and HNO_3 (about –200 kJ/mole) are somewhat large and negative. These propellants are used only when high performance is not a requirement.

The oxygen content in HNO_3 is enhanced by dissolving about 15 per cent NO_2 in it. Red fumes are obtained from the high NO_2 content and the mixture is known as Red Fuming Nitric Acid (RFNA). The incorporation of a small quantity of NO_2 content in HNO_3 (about 0.5 per cent) is known as White Fuming Nitric Acid (WFNA).

HNO_3 is very corrosive. The addition of about 0.5 to 0.8 per cent of hydrofluoric acid (HF) to RFNA inhibits the corrosion of the storage vessel and the inhibited RFNA is termed as Inhibited Red Fuming Nitric Acid (IRFNA). IRFNA with aniline and xylidine have been extensively used in the past especially for low performing missiles.

Fuel hydrazine (N_2H_4) has a much simpler molecular structure with bonds as illustrated below:



It has a positive heat of formation and dissociates in the presence of a catalyst to liberate heat. It is, therefore, sometimes used as a single propellant without the need for an oxidiser and is, therefore, called a monopropellant. Similarly, the oxidiser hydrogen peroxide (H_2O_2) liberates heat during its decomposition and can be used as a monopropellant. N_2H_4 combines readily with oxidisers, such as, HNO_3 and N_2O_4 giving much higher heat release than RFNA with aniline and xylidine and forms combustion products with lower molecular mass.

Medium-energy Propellants

The use of UDMH, N_2H_4 and Az50 with LO_2 gives sea-level I_{sp} between 3,000 and 3,500 Ns/kg. The use of kerosene with liquid Fluorine, which is an extremely reactive oxidiser also provides the higher sea-level I_{sp} between 3,000 and 3,500 Ns/kg. Such of the propellant combinations having I_{sp} in this range are known as medium energy propellants. The medium energy propellants are not popular and only UDMH-LO_2 combination has been used in practice. The use of Fluorine has been difficult in view of its toxicity and reactivity.

High-energy Propellants

High energy propellants have sea-level I_{sp} greater than 4000 Ns/kg. Two propellant combinations comprising Liquid Hydrogen (LH_2) with LO_2 and with Liquid Fluorine (LF) fall in this category. Hydrogen contributes to a significantly reduced molecular mass of the combustion gases. Since LH_2, LO_2 and LF are liquids only at cryogenic temperatures, these propellant combinations [LH_2/LO_2, LH_2/LF] are known as cryogenic propellants. The boiling point of LF is about 5°C lower than LO_2. LF is seldom used for reasons of reactivity cited earlier. The only high energy propellant used in practice is LH_2-LO_2.

VARIOUS COMBUSTION MODELS:

- Gas Phase Governing Equation
- Liquid Particle Trajectory Model
- Turbulence Model
- Droplets Atomizing Model
- Droplet Evaporation Model

- Chemical Reaction Kinetics Model

Gas Phase Conservation Equations

Based on the assumptions, the mass, energy, and components conservation equations for droplet evaporation at spherical coordinates can be obtained

$$\dot{m} = 4\pi r^2 \rho v = 4\pi r^2 \rho_s v_s$$

$$r^2 \rho v c_p \frac{\mathrm{d}T}{\mathrm{d}r} = \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \lambda \frac{\mathrm{d}T}{\mathrm{d}r}\right)$$

$$r^2 \rho v \frac{\mathrm{d}Y_F}{\mathrm{d}r} = \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Y_F}{\mathrm{d}r}\right)$$

$\dot{m}$ is the droplet evaporation rate;
r is the radius of spherical coordinates;
ρ and v are the density and velocity, respectively, of the mixture of ambient gas and droplet vapor at r;
T is the temperature of the gaseous mixture;
c_p is the specific heat capacity;
Y_F is the mass fraction of the droplet vapor in the mixture;
D is the diffusion coefficient;
the subscript s denotes the droplet surface.

Liquid Particle Trajectory Models

A liquid rocket engine spray combustion process is a typical process of two phase flow. At present, two-phase flow models mainly include the single fluid model, particle trajectory model, and quasi fluid model. The particle trajectory model is the most widely used in numerical calculations of the liquid rocket engine combustion process. Based on the particle track model assumptions, the gas is treated as continuum and the droplet groups are treated as a discrete system.

In the particle trajectory model, the trajectory of discrete phase particles (droplets) is obtained by integrating the differential equation of the particles forces in Lagrangian coordinates. The particles balance equations are:

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{V}_p$$

$$\frac{\mathrm{d}\vec{V}_p}{\mathrm{d}t} = F_D\left(\vec{V} - \vec{V}_p\right) + \frac{\vec{g}(\rho_p - \rho)}{\rho_p} + \vec{F}$$

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \mathrm{Re}}{24}$$

$\vec{V}$ is the gas phase velocity;
$\vec{V}_p$ is the particle velocity;
μ is the viscosity of fluid dynamics;
ρ is fluid density;
ρ_p is the particle density;
d_p is the particle diameter;
$\vec{g}$ is the acceleration due to gravity;
$\vec{F}$ represents all the other forces, including Stefan flow, the pressure gradient force, and other volume forces;
$F_D\left(\vec{V} - \vec{V}_p\right)$ is the resistance of the particle per unit mass;
C_D is the coefficient of the resistance.

Assuming that each droplet is a round ball, C_D can adopt the following expression:

$$C_D = \frac{24}{\mathrm{Re}}\left(1 + b_1 \mathrm{Re}^{b_2}\right) + \frac{b_3 \mathrm{Re}}{b_4 + \mathrm{Re}}$$

In the formula, the shape factor ϕ is defined as follows:

$$\phi = \frac{s}{S}$$

where s is the spherical particle surface area, which has the same volume as the actual particle, and S is the actual particle surface area.

$$S_{\mathrm{d,m}} = \frac{\Delta m_{\mathrm{d}}}{m_{\mathrm{d},0}} \dot{m}_{\mathrm{d},0}$$

The Mass equation

The momentum:

$$\vec{S}_{\mathrm{d,v}} = \left(\frac{18 \mu C_D \mathrm{Re}}{\rho_{\mathrm{d}} d_{\mathrm{d}}^2 24}\left(\vec{V} - \vec{V}_{\mathrm{d}}\right) + \vec{F}_x\right) \dot{m}_{\mathrm{d}} \Delta t$$

The energy:

$$S_{\mathrm{d,h}} = \left[\frac{\bar{m}_{\mathrm{d}}}{m_{\mathrm{d},0}} c_{\mathrm{drop}} \Delta T_{\mathrm{d}} + \frac{\Delta m_{\mathrm{d}}}{m_{\mathrm{d},0}}\left(-h_{\mathrm{fg}} + h_{\mathrm{pyrol}} + \int_{T_{\mathrm{ref}}}^{T_{\mathrm{d}}} C_{p,1} \mathrm{d}T\right)\right] \dot{m}_{\mathrm{d},0}$$

Δm_{d} is the change of the unit mass of the droplets through the control unit;
$m_{\mathrm{d},0}$ is the initial mass;
$\dot{m}_{\mathrm{d},0}$ is the initial mass flow rate;
$\dot{m}_{\mathrm{d}}$ is the mass flow rate of the droplet;
Δt is the time step in the calculation;
$\bar{m}_{\mathrm{d}}$ is the average mass of the droplet in a grid cell in calculation;
ΔT_{d} is the change of droplet temperature in grid cell in calculation;
h_{fg} is the latent heat of vaporization of the fuel droplet;

Turbulence Model

Based on the Boussinesq hypothesis, in the gas phase governing equations, the viscosity coefficient (μ) can be decomposed into the laminar viscous coefficient (μl) and the turbulent viscosity coefficient (μt: μ = μl + μt). Among them, μl is given by the Sutherland formula:

$$\mu_1 = \mu_{\mathrm{ref}} (T/T_{\mathrm{ref}})^{3/2} (T_{\mathrm{ref}} + S_{\mathrm{T}})/(T + S_{\mathrm{T}})$$

In the formula, T_{ref} is the reference temperature, S_{T} is the equivalent temperature, and μ_{ref} is the reference viscosity coefficient corresponding to T_{ref}.

$$\frac{\partial}{\partial t}(\bar{\rho}k)+\frac{\partial}{\partial x_i}(\bar{\rho}k\widetilde{u}_i)=\frac{\partial}{\partial x_j}\left(\Gamma_k\frac{\partial k}{\partial x_j}\right)+2\mu_t\bar{S}_{ij}\bar{S}_{ij}-\bar{\rho}\beta^* f_{\beta^*}\omega$$

$$\frac{\partial}{\partial t}(\bar{\rho}\omega)+\frac{\partial}{\partial x_i}(\bar{\rho}\omega\widetilde{u}_i)=\frac{\partial}{\partial x_j}\left(\Gamma_\omega\frac{\partial \omega}{\partial x_j}\right)+2\frac{\omega}{k}\mu_t\bar{S}_{ij}\bar{S}_{ij}-\bar{\rho}\beta f_\beta\omega^2$$

In the formula,

$$\Gamma_k=\mu_1+\frac{\mu_t}{\sigma_k}\,\Gamma_\omega=\mu_1+\frac{\mu_t}{\sigma_\omega}\mu_t=\frac{\bar{\rho}k}{\omega}$$

$$\mu_t=\rho L_s^2|\bar{S}| \qquad |\bar{S}|=\sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$$

$$\bar{S}_{ij}=\frac{1}{2}\left(\frac{\partial\widetilde{u}_i}{\partial x_j}+\frac{\partial\widetilde{u}_j}{\partial x_i}\right)$$

L_s is the mixing length of the sub-grid: $L_s=\min\left(\kappa d, C_s V^{1/3}\right)$

κ is the von Karman constant,
d is the nearest distance to the wall,
C_s is the Smagorinsky constant,
V is the volume of the cell.

Droplets Atomizing Model:

In numerical calculations of the liquid rocket engine combustion process, the spray model as the initial and boundary conditions of the spray combustion calculation has an important influence on the calculation results.

The spray model includes spray size distribution model, the flow intensity distribution model, and mixing ratio distribution model, respectively obtaining the mean diameter distribution of spray droplets, the position distribution of droplets, and the initial velocity distribution of droplets.

As the atomization process is more complicated, we usually do not consider the details of the liquid atomization process. Instead, for the injector used in the experiments, the distribution characteristics of droplets (including parameters such as droplet size distribution, velocity distribution, and temperature) are directly given based on experimental results in combination with the empirical formula to directly simulate the liquid atomization result.

Droplet Evaporation Model:

The internal flow and heat transfer process of the droplet usually have two limit cases, which are known as the surface model and the uniform temperature model. The surface model assumes that the coefficient of temperature conductivity of the fuel droplet α 0, assuming that a high temperature difference always exists between the surface of a drop and its internal mass.

Assuming that the droplet internal temperature is equal to the initial droplet temperature, only the droplet surface temperature reaches the thermodynamic equilibrium temperature, and the droplet can exchange heat and mass with external air flow through the surface. The surface model is used in the treatment of droplet evaporation in still air. The uniform temperature model is also known as the infinite thermal conductivity model.

It assumes that the coefficient of temperature conductivity of the drop α ∞, and that the droplet internal circulation and other factors mean that the droplet temperature is always uniform and identical to the surface temperature. This model is applicable to the droplet evaporation of small droplets, strong convection, and when the droplet internal circulation is good.

When we deal with the droplet preheating problem, surface models usually ignore droplet evaporation in the heating period, and the droplet internal heating is calculated according to the unsteady heat conduction. When the droplet surface temperature reaches the equilibrium temperature, the evaporation where the heat and mass transfer are balanced between the two phases is established.

The uniform temperature model assumes that the droplet evaporation is determined by the diffusion in the droplet preheating period, which is a non-equilibrium evaporation process; the heat transmitted to the droplet not only heats the droplet but also provides the heat required for droplet evaporation; After reaching the equilibrium temperature, we have a stable evaporation process when the diffusion and heat transfer is in phase equilibrium.

The equilibrium temperature of droplet steady evaporation is closely related to the flow conditions, usually growing with increasing flow temperature. When the current temperature is extremely high, the equilibrium temperature will be close to the boiling temperature of liquid drops. Unlike the model of droplet evaporation in static air, a droplet undergoes deformation due to the ambient air flow effect in convection conditions.

Chemical Reaction Kinetics Model:

For a chemical reaction system composed of N_R reactions, the production rate of component i is

$$\omega_i = M_{\mathrm{w},i} \sum_{r=1}^{N_\mathrm{R}} \hat{\omega}_{i,r}$$

where $\hat{\omega}_{i,r}$ is the Arrhenius molecular production rate of component i in the r-th reaction and $M_{\mathrm{w},i}$ is the molecular weight of component i.

The general form of the r-th reaction equation is:

$$\sum_{i=1}^{N} \nu'_{i,r} M_i \overset{k_{\mathrm{f},r}}{\underset{k_{\mathrm{b},r}}{\Leftrightarrow}} \sum_{i=1}^{N} \nu''_{i,r} M_i$$

N is the total component number of the reaction;
$\nu'_{i,r}, \nu''_{i,r}$ represent the stoichiometric coefficients of the chemical component i in the positive and reverse reactions, respectively;
M_i is the molecular weight of chemical component i;
$k_{\mathrm{f},r}, k_{\mathrm{b},r}$ is the rate constants of the positive and reverse reaction.

Theory for Quasi-Steady Evaporation and Combustion of a Single Droplet at Atmospheric Pressure:

It is also assumed that the droplets contain only one chemical component. Moreover, in most cases there is a velocity difference between the droplets and the ambient gas during combustion, and thus the effect of convective heat and mass transfer on the droplet evaporation rate should be examined. This section first describes droplet evaporation and the combustion process in a static environment, and then analyzes droplet evaporation and combustion in the case of convection.

Consider the evaporation of an isolated droplet in a static gas without combustion (Figure). The initial droplet temperature is T_0 and the temperature of the ambient gas is T_∞ . To simplify the analysis, the following assumptions are introduced:

1. There is only spherically one-dimensional flow caused by the Stefan flow around the droplet, and the spherically symmetric center is the center of the spherical droplet.
2. The gas flow field is quasi-steady with a constant pressure.
3. The gas is immiscible with the liquid droplet.
4. Droplets contains only one component, the internal temperature is uniform and equal to the initial temperature, and the surface of the two phases is at equilibrium.
5. The gas phase Lewis number (Le) is 1.
6. The physical properties of the flow field (thermal conductivity coefficient (λ), specific heat capacity (cp), and ρD where D is the gas mass diffusion coefficient) are assumed to be constant.

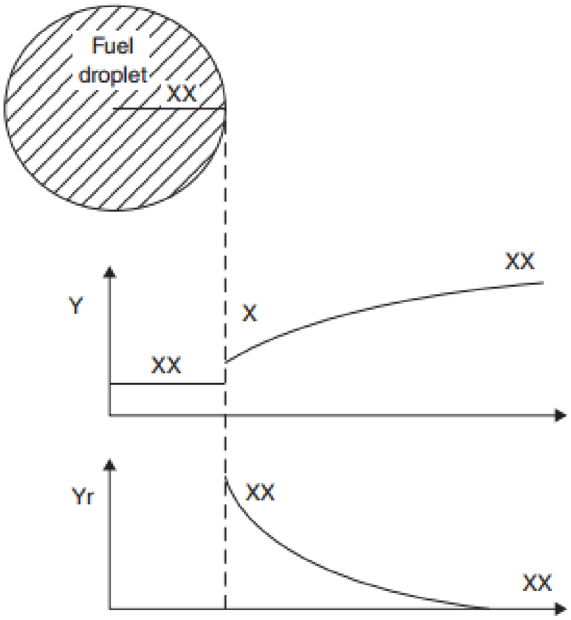


Fig. Quasi-steady evaporation model for a droplet in a static gas without combustion.

Gas Phase Conservation Equations

Based on the assumptions, the mass, energy, and components conservation equations for droplet evaporation at spherical coordinates can be obtained

$$\dot{m} = 4\pi r^2 \rho v = 4\pi r^2 \rho_s v_s$$

$$r^2 \rho v c_p \frac{dT}{dr} = \frac{d}{dr}\left(r^2 \lambda \frac{dT}{dr}\right)$$

$$r^2 \rho v \frac{dY_F}{dr} = \frac{d}{dr}\left(r^2 \rho D \frac{dY_F}{dr}\right)$$

$\dot{m}$ is the droplet evaporation rate;
r is the radius of spherical coordinates;
ρ and v are the density and velocity, respectively, of the mixture of ambient gas and droplet vapor at r;
T is the temperature of the gaseous mixture;
c_p is the specific heat capacity;
Y_F is the mass fraction of the droplet vapor in the mixture;
D is the diffusion coefficient;
the subscript s denotes the droplet surface.

Equation Solutions:

Distribution of Droplet Vapor Concentration Assuming that:

$$b = \frac{Y_F}{Y_{Fs} - 1},$$ wkt,

$$r^2 \rho v \frac{db}{dr} = \frac{d}{dr}\left(r^2 \rho D \frac{db}{dr}\right)$$

The boundary conditions are as follows: At $r = r_s$: $\left(\frac{db}{dr}\right)_s = \frac{v_s}{D_s}$ At $r \to \infty$: $b = b_\infty = \frac{Y_{F\infty}}{Y_{Fs} - 1}$

The following correlation can be derived by integrating Equation

$$r_s^2 \rho_s v_s (b - b_s) = r^2 \rho D \frac{db}{dr} - r_s^2 \rho_s D_s \left(\frac{db}{dr}\right)_s$$

Substituting Equation into above the following equation can be obtained:

$$r_s^2 \rho_s v_s (b - b_s + 1) = r^2 \rho D \frac{db}{dr}$$

From assumptions

$$-\frac{r_s^2 v_s}{D_s} d\left(\frac{1}{r}\right) = \frac{db}{(b - b_s + 1)}$$

$$\frac{r_s^2 v_s}{r D_s} = \ln\left(\frac{b_\infty - b_s + 1}{b - b_s + 1}\right)$$

Since the droplet surface parameters are known, the above equation describes the relation between the droplet vapor concentration and radius. The vapor concentration declines exponentially with the radius.

At r = rs

$$\frac{r_s v_s}{D_s} = \ln(b_\infty - b_s + 1) = \ln(1 + B_m)$$

where,

$$B_m = b_\infty - b_s = \frac{Y_{Fs} - Y_{F\infty}}{1 - Y_{Fs}}$$

which is called the Spalding transfer function. The relation between the mixture velocity and vapor concentration on the droplet surface can be derived from Equation 3.11.

$$v_s = \frac{D_s \ln(1 + B_m)}{r_s}$$

The droplet mass consumption rate can be computed by

$$\dot{m} = -4\pi r_s^2 \rho_l \frac{dr_s}{dt} = -\frac{\pi}{4} d_s \rho_l \frac{d(d_s^2)}{dt}$$

where ρl is the density of the droplet. Since the droplet evaporation rate is equal to the consumption rate, the following correlation can be derived:

$$\frac{d(d_s^2)}{dt} = -\frac{8\rho_s D_s}{\rho_l} \ln(1 + B_m) = -K$$

where K is the evaporation constant, which is proportional to the transport coefficient ρD. By integrating above Equation, the following correlation can be obtained,

$d_s^2 = d_0^2 - Kt$ where d_0 is the initial droplet diameter.

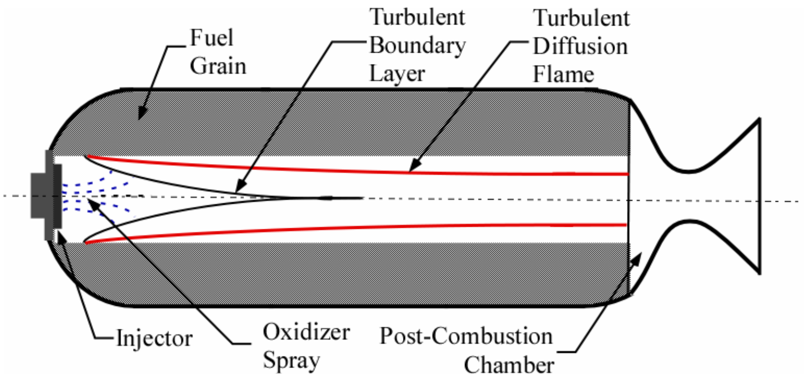
The time required for droplet evaporation can be computed by

$$t_v = \frac{d_0^2}{K}$$

Therefore, a bigger droplet would take longer to finish the evaporation process.

COMBUSTION IN HYBRID ROCKETS:

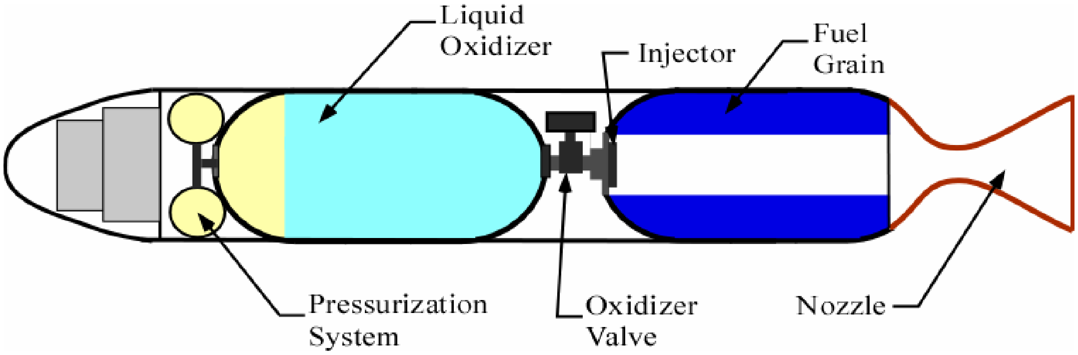
Hybrid Rocket System



Solid Fuel • Polymers: Thermoplastics, (Polyethylene, Plexiglas), Rubbers (HTPB) • Wood, Trash, Wax

Liquid Oxidizer • Cryogenic: LO_2 • Storable: H_2O_2, N_2O, N_2O

Hybrid Rocket Configuration:



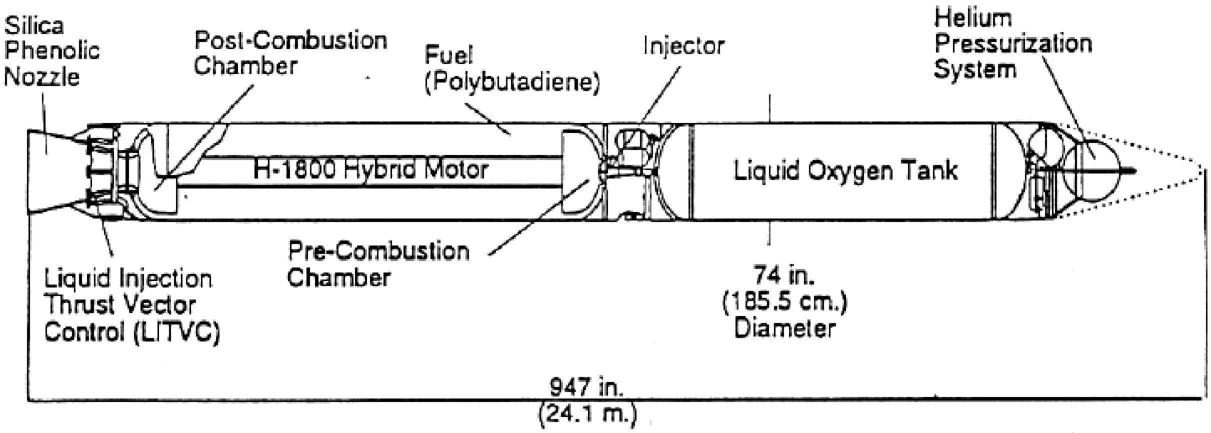
Fuel and oxidizer are physically separated One of the two is in solid phase.

Most Hybrids: Reverse Hybrids: Oxidizer: Solid ,Fuel: Liquid

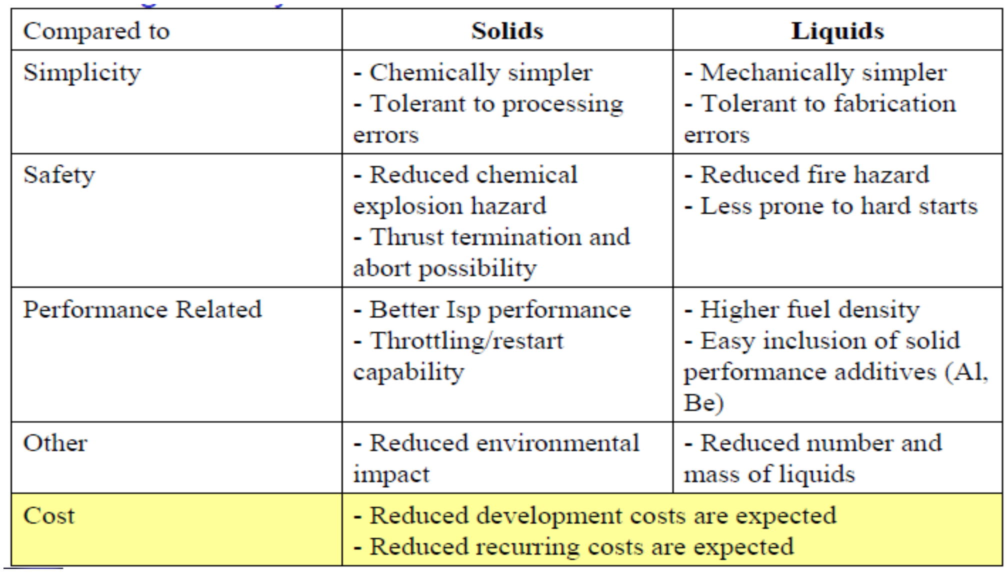
Oxidizer: Liquid

Fuel: Solid

Hybrid Rocket Configuration-AMROC Booster:



Advantages of Hybrids:



Compared to	**Solids**	**Liquids**
Simplicity	- Chemically simpler - Tolerant to processing errors	- Mechanically simpler - Tolerant to fabrication errors
Safety	- Reduced chemical explosion hazard - Thrust termination and abort possibility	- Reduced fire hazard - Less prone to hard starts
Performance Related	- Better Isp performance - Throttling/restart capability	- Higher fuel density - Easy inclusion of solid performance additives (Al, Be)
Other	- Reduced environmental impact	- Reduced number and mass of liquids
Cost	- Reduced development costs are expected - Reduced recurring costs are expected	

UNIT –V

SUPERSONIC COMBUSTION

Introduction to Supersonic combustion

A scramjet ("supersonic combustion ramjet") is a variant of a ramjet airbreathing jet engine in which combustion takes place in supersonic airflow. As in ramjets, a scramjet relies on high vehicle speed to compress the incoming air forcefully before combustion (hence ramjet), but whereas a ramjet decelerates the air to subsonic velocities before combustion, the airflow in a scramjet is supersonic throughout the entire engine. That allows the scramjet to operate efficiently at extremely high speeds.

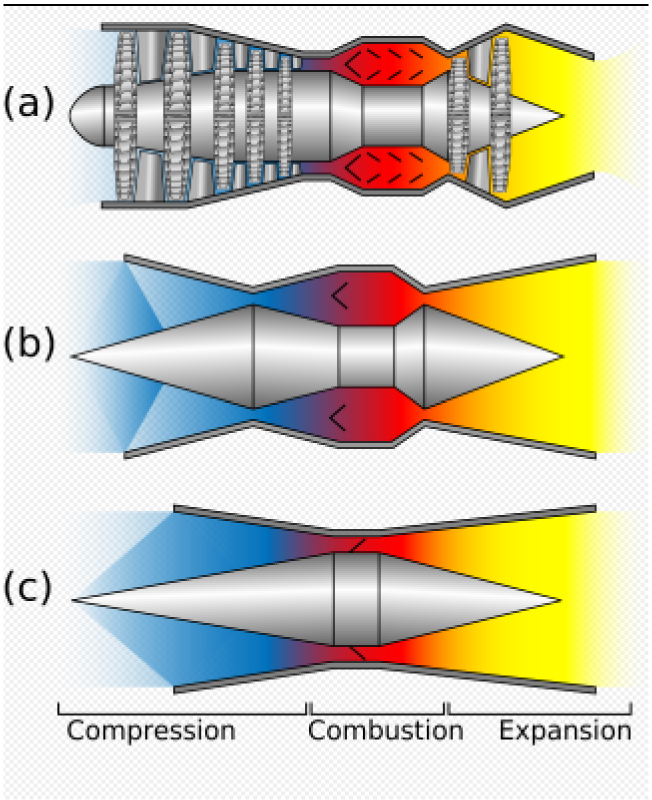
Basic principles

The compression, combustion, and expansion regions of: (a) turbojet, (b) ramjet, and (c) scramjet engines.

Scramjets are designed to operate in the hypersonic flight regime, beyond the reach of turbojet engines, and, along with ramjets, fill the gap between the high efficiency of turbojets and the high speed of rocket engines. Turbo machinery-based engines, while highly efficient at subsonic speeds, become increasingly inefficient at transonic speeds, as the compressor rotors found in turbojet engines require subsonic speeds to operate. While the flow from transonic to low supersonic speeds can be decelerated to these conditions, doing so at supersonic speeds results in a tremendous increase in temperature and a loss in the total pressure of the flow. Around Mach 3–4, turbo machinery is no longer useful, and ram-style compression becomes the preferred method.

Ramjets utilize high-speed characteristics of air to literally 'ram' air through an inlet diffuser into the combustor. At transonic and supersonic flight speeds, the air upstream of the inlet is not able to move out of the way quickly enough, and is compressed within the diffuser before being diffused into the combustor. Combustion in a ramjet takes place at subsonic velocities, similar to turbojets, but the combustion products are then accelerated through a convergent-divergent nozzle to supersonic speeds. As they have no mechanical means of compression, ramjets cannot start from a standstill, and generally do not achieve sufficient compression until supersonic flight. The lack of intricate turbo machinery allows ramjets to deal with the temperature rise associated with decelerating a supersonic flow to subsonic speeds, but this only goes so far: at near-hypersonic velocities, the temperature rise and inefficiencies discourage decelerating the flow to the magnitude found in ramjet engines.

Scramjet engines operate on the same principles as ramjets, but do not decelerate the flow to subsonic velocities. Rather, a scramjet combustor is supersonic: the inlet decelerates the flow to a lower Mach number for combustion, after which it is accelerated to an even higher Mach number through the nozzle. By limiting the amount of deceleration, temperatures within the engine are kept at a tolerable level, from both a material and combustive standpoint. Even so, current scramjet technology requires the use of high-energy fuels and active cooling schemes to maintain sustained operation, often using hydrogen and regenerative cooling techniques



Advantages and disadvantages of scramjets

Advantages

Does not have to carry oxygen

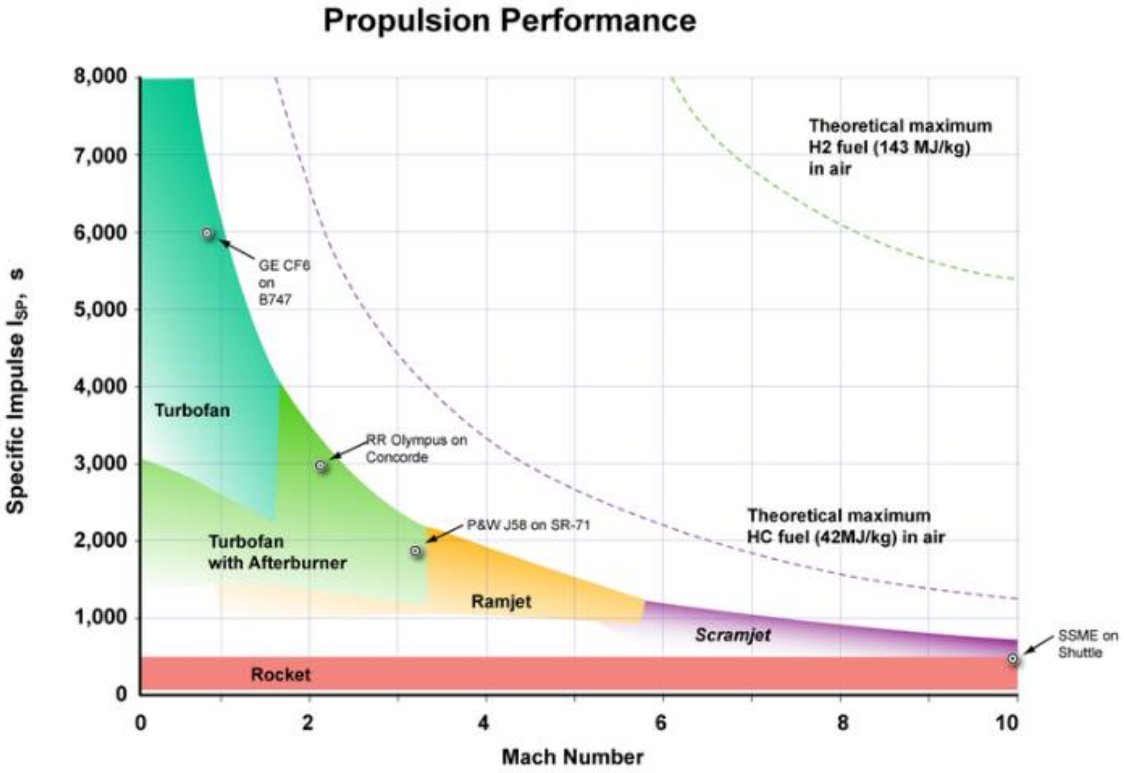
No rotating part makes it easier to manufacture than a turbojet

Has a higher specific impulse (change in momentum per unit of propellant) than a rocket engine; could provide between 1000 and 4000 seconds, while a rocket typically provides around 450 seconds or less. Higher speed could mean cheaper access to outer space in the future

Special cooling and materials

Unlike a rocket that quickly passes mostly vertically through the atmosphere or a turbojet or ramjet that flies at much lower speeds, a hypersonic air breathing vehicle optimally flies a "depressed trajectory", staying within the atmosphere at hypersonic speeds. Because scramjets have only mediocre thrust-to-weight ratios, acceleration would be limited. Therefore, time in the atmosphere at supersonic speed would be considerable, possibly 15–30 minutes. Similar to a reentering space vehicle, heat insulation would be a formidable task, with protection required for duration longer than that of a typical space capsule, although less than the space shuttle.

Vehicle performance



The performance of a launch system is complex and depends greatly on its weight. Normally craft are designed to maximise range (R), orbital radius (R) or payload mass fraction (ŕ) for a given engine and fuel. This results in tradeoffs between the efficiency of the engine (takeoff fuel weight) and the complexity of the engine (takeoff dry weight), which can be expressed by the following:

$$\Pi_e + \Pi_f + \frac{1}{\Gamma} = 1$$

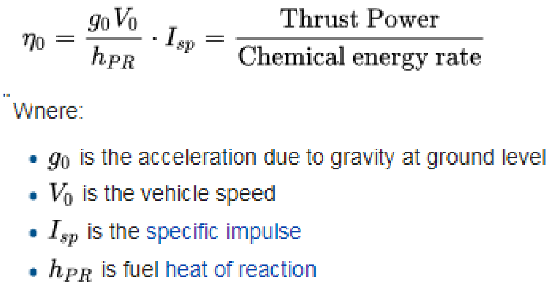
where

- $\Pi_e = \frac{m_{\text{empty}}}{m_{\text{initial}}}$ is the empty mass fraction, and represents the weight of the superstructure, tankage and engine.
- $\Pi_f = \frac{m_{\text{fuel}}}{m_{\text{initial}}}$ is the fuel mass fraction, and represents the weight of fuel, oxidiser and any other materials which are consumed during the launch.
- $\Gamma = \frac{m_{\text{initial}}}{m_{\text{payload}}}$ is initial mass ratio, and is the inverse of the payload mass fraction. This represents how much payload the vehicle can deliver to a destination.

A scramjet increases the mass of the motor Π_e over a rocket, and decreases the mass of the fuel Π_f. It can be difficult to decide whether this will result in an increased ŕ (which would be an increased payload delivered to a destination for a constant vehicle takeoff weight).

For an engine strongly integrated into the aerodynamic body, it may be more convenient to think of $\mathbf{D_e}$ as the difference in drag from a known base configuration.

The overall engine efficiency can be represented as a value between 0 and 1 ƞ, in terms of the specific impulse of the engine:

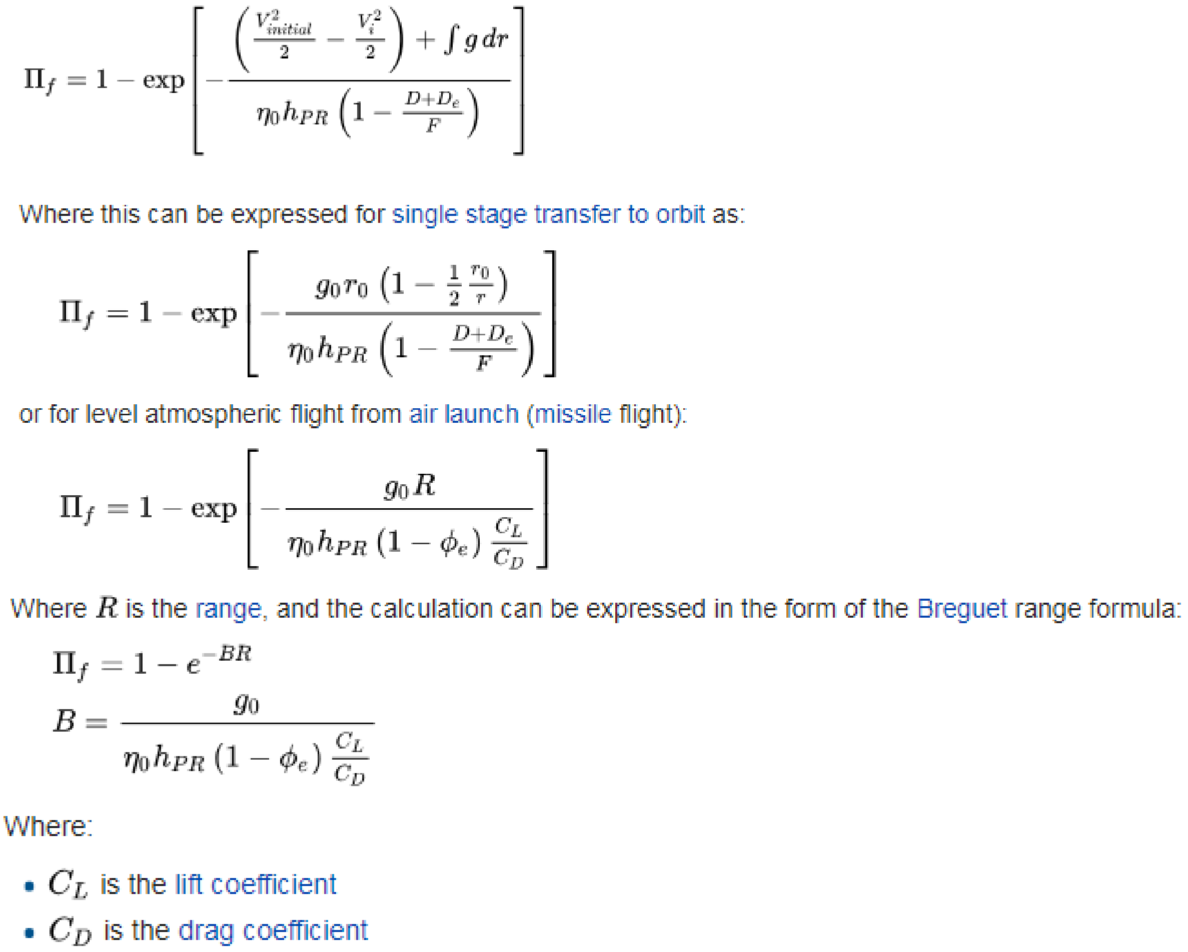


$$\eta_0 = \frac{g_0 V_0}{h_{PR}} \cdot I_{sp} = \frac{\text{Thrust Power}}{\text{Chemical energy rate}}$$

Where:

- g_0 is the acceleration due to gravity at ground level
- V_0 is the vehicle speed
- I_{sp} is the specific impulse
- h_{PR} is fuel heat of reaction

Specific impulse is often used as the unit of efficiency for rockets, since in the case of the rocket, there is a direct relation between specific impulse, specific fuel consumption and exhaust velocity. This direct relation is not generally present for air breathing engines, and so specific impulse is less used in the literature. Note that for an air breathing engine, both ƞ and I_{sp} are a function of velocity.



$$\Pi_f = 1 - \exp\left[-\frac{\left(\frac{V_{initial}^2}{2} - \frac{V_i^2}{2}\right) + \int g\,dr}{\eta_0 h_{PR}\left(1 - \frac{D+D_e}{F}\right)}\right]$$

Where this can be expressed for single stage transfer to orbit as:

$$\Pi_f = 1 - \exp\left[-\frac{g_0 r_0 \left(1 - \frac{1}{2}\frac{r_0}{r}\right)}{\eta_0 h_{PR}\left(1 - \frac{D+D_e}{F}\right)}\right]$$

or for level atmospheric flight from air launch (missile flight):

$$\Pi_f = 1 - \exp\left[-\frac{g_0 R}{\eta_0 h_{PR}\left(1 - \phi_e\right)\frac{C_L}{C_D}}\right]$$

Where R is the range, and the calculation can be expressed in the form of the Breguet range formula:

$$\Pi_f = 1 - e^{-BR}$$

$$B = \frac{g_0}{\eta_0 h_{PR}\left(1 - \phi_e\right)\frac{C_L}{C_D}}$$

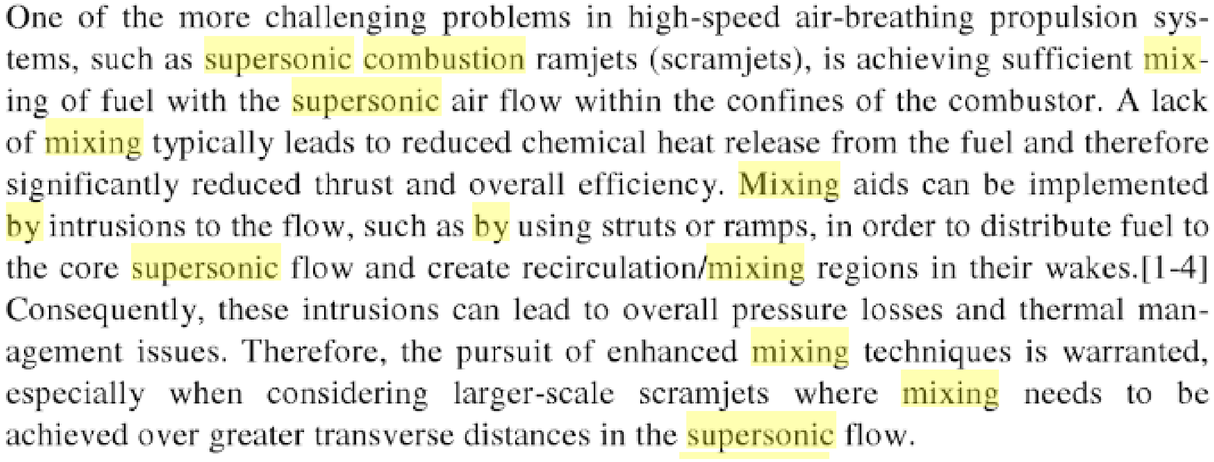
Where:

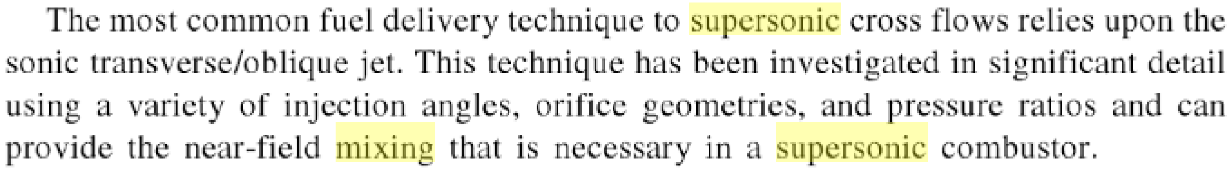
- C_L is the lift coefficient
- C_D is the drag coefficient

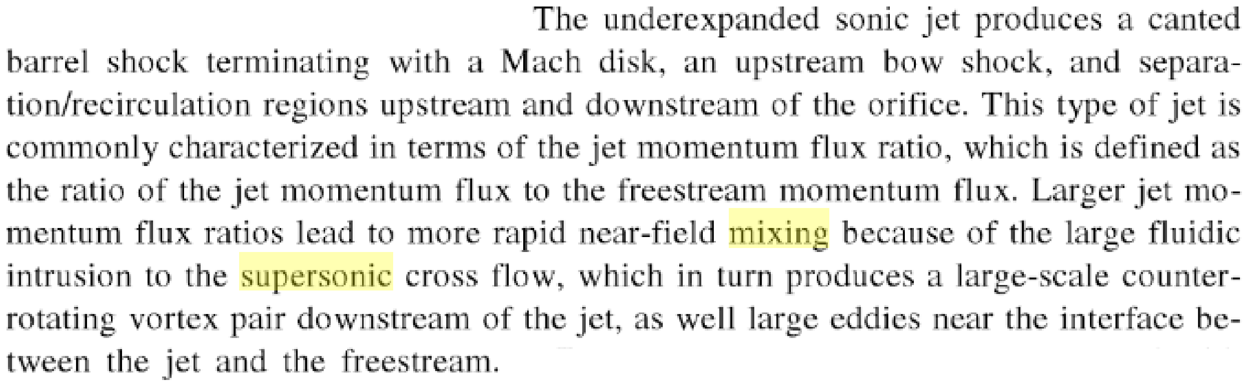
Disadvantages

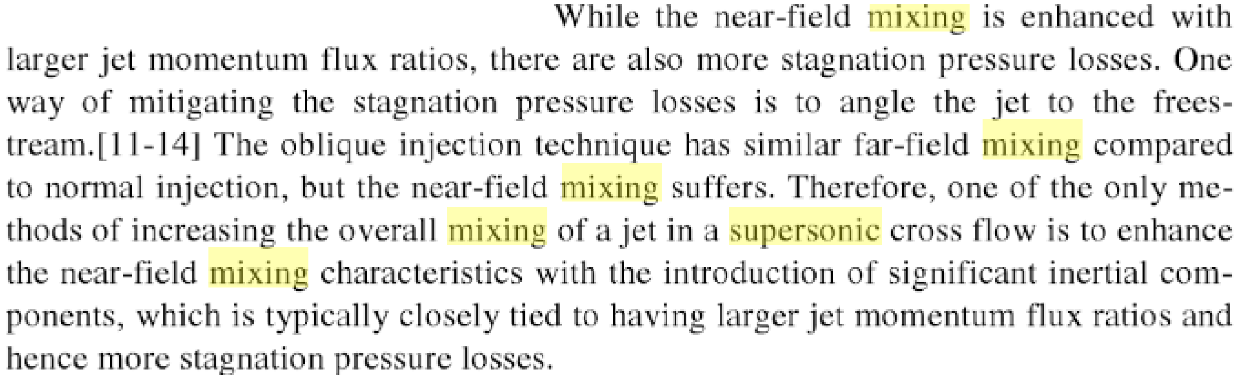
- Difficult / expensive testing and development
- Very high initial propulsion requirements

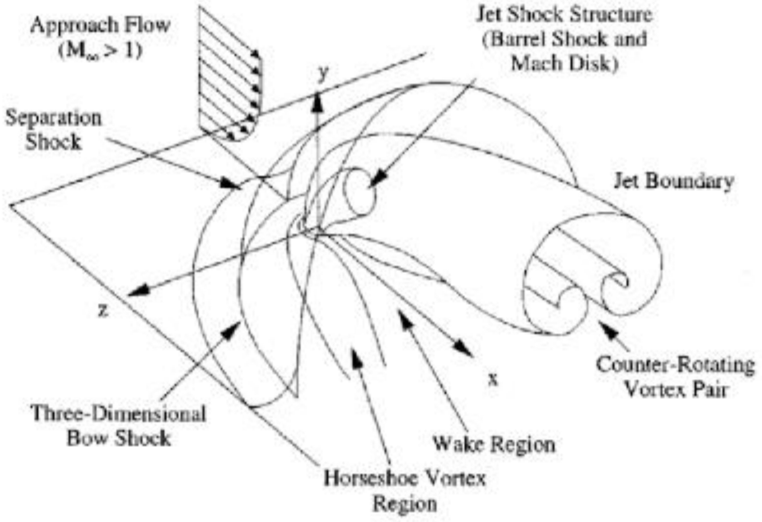
Supersonic combustion controlled by Mixing


One of the more challenging problems in high-speed air-breathing propulsion systems, such as supersonic combustion ramjets (scramjets), is achieving sufficient mixing of fuel with the supersonic air flow within the confines of the combustor. A lack of mixing typically leads to reduced chemical heat release from the fuel and therefore significantly reduced thrust and overall efficiency. Mixing aids can be implemented by intrusions to the flow, such as by using struts or ramps, in order to distribute fuel to the core supersonic flow and create recirculation/mixing regions in their wakes.[1-4] Consequently, these intrusions can lead to overall pressure losses and thermal management issues. Therefore, the pursuit of enhanced mixing techniques is warranted, especially when considering larger-scale scramjets where mixing needs to be achieved over greater transverse distances in the supersonic flow.


The most common fuel delivery technique to supersonic cross flows relies upon the sonic transverse/oblique jet. This technique has been investigated in significant detail using a variety of injection angles, orifice geometries, and pressure ratios and can provide the near-field mixing that is necessary in a supersonic combustor.


The underexpanded sonic jet produces a canted barrel shock terminating with a Mach disk, an upstream bow shock, and separation/recirculation regions upstream and downstream of the orifice. This type of jet is commonly characterized in terms of the jet momentum flux ratio, which is defined as the ratio of the jet momentum flux to the freestream momentum flux. Larger jet momentum flux ratios lead to more rapid near-field mixing because of the large fluidic intrusion to the supersonic cross flow, which in turn produces a large-scale counter-rotating vortex pair downstream of the jet, as well large eddies near the interface between the jet and the freestream.


While the near-field mixing is enhanced with larger jet momentum flux ratios, there are also more stagnation pressure losses. One way of mitigating the stagnation pressure losses is to angle the jet to the freestream.[11-14] The oblique injection technique has similar far-field mixing compared to normal injection, but the near-field mixing suffers. Therefore, one of the only methods of increasing the overall mixing of a jet in a supersonic cross flow is to enhance the near-field mixing characteristics with the introduction of significant inertial components, which is typically closely tied to having larger jet momentum flux ratios and hence more stagnation pressure losses.



Supersonic combustion controlled by Diffusion

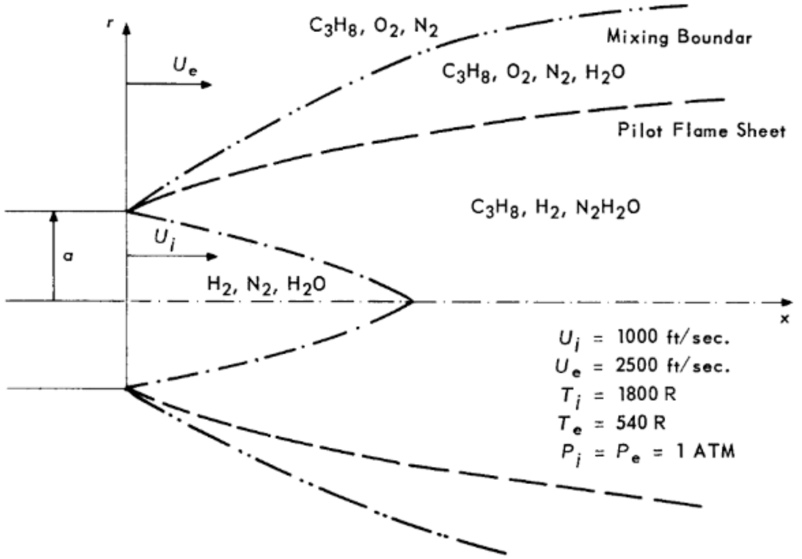
The aerodynamic design of a combustor in scramjet speed is related to two basic problems: mixing and combustion. Two different effects produced by the mixing of two jets can be used to control the supersonic combustion, depending on the static conditions of the jets before combustion. When the static pressure and temperature of the two mixing streams are sufficiently high so that chemical reaction rates are fast, the diffusion of one species in the other produced by the mixing is used, *e.g.*, for a controlling mechanism for combustion. This type of control is used in the higher range of flight Mach numbers and is the type considered in References 2, 7 and 8. When the static temperature and pressure of the two mixing streams are low, supersonic combustion can still take place, but it must be controlled by the heat convection produced by mixing and needs some kind of pilot flame. This second process is important because it extends the possibility of using supersonic combustion for ramjets into the lower range of Mach numbers.

Supersonic combustion controlled by heat convection

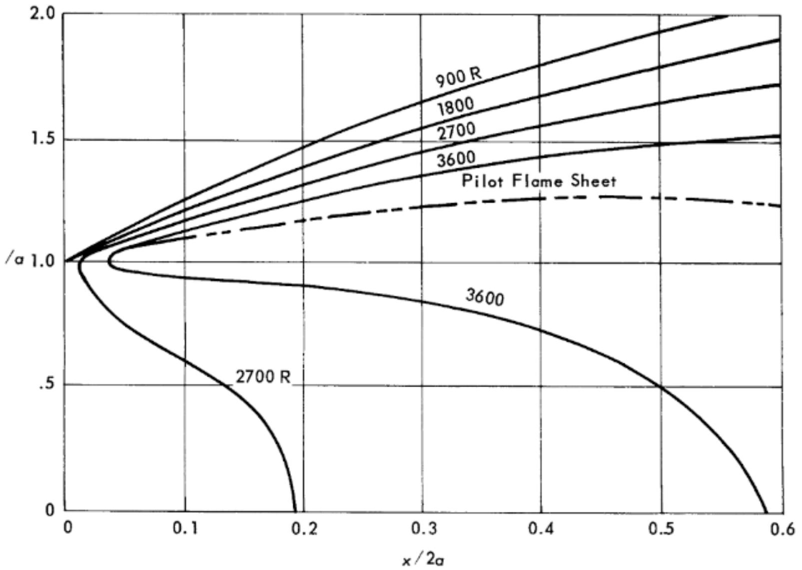
The heat convection process produced by mixing can be used in place of the diffusion process as a controlling mechanism for a supersonic flame. To illustrate this concept, consider a small jet of gas having very high static temperature and discharging in a flow having high velocity and low static temperature (Fig. 14-7). For simplicity, assume that the two gases are at the same pressure. Because of the mixing process, the concentration of the two gases changes gradually and the static temperature changes. The gas from the external jet mixes with the hot gas and is heated while the gas from the central jet is cooled. If the mixing takes place without chemical reaction, the temperature at the axis of the jet gradually decreases.

However, if the gas of the external jet is a premixed reacting mixture and the temperature of the central jet is sufficiently high, then because of the heating process due to mixing, the external gas reacts and combustion takes place. The heat released by the reacting gases tends to keep up the temperature of the central core of the flow and, if the balance of heat is favorable, the combustion continues while mixing takes place and propagates towards the external flow. The propagation is controlled by the heat convection related to the mixing process. The example presented in Fig. 14-7

The mechanism of combustion described here is of practical importance because it permits us to produce combustion in flows having static temperatures below the temperature required for rapid ignition and, therefore, extends the possibility of using supersonic combustion controlled by mixing in the range of flight Mach numbers below 6 or 7. This scheme also allows the possibility



Schematic of ignition of propane-air mixture with hydrogen-air pilot.



Isotherms and pilot flame sheet.

of supersonic combustion with fuels having very long reaction times at the static temperature and pressure existing in the burner of the engine for the flight conditions considered. The propane-air reaction for the conditions assumed in Fig.

SUPERSONIC BURNING WITH DETONATION SHOCKS.

The shock that is the precursor to the combustion front in a detonation wave is taken to be infinitesimal in most applications. The width of the burning region that follows the shock in a detonation, known as the *induction length*, is $L_{in} \sim S_{sh}\tau$, where S_{sh} is the shock speed and τ is the timescale for the reaction, known as the *induction time*. For chemical reactions, the induction time can be a complicated function, but for nuclear reactions where the burning rate is generally monotonic with ρ, T, and fuel composition, the induction time, while very rapid, can be straightforwardly defined as the time to burn some fraction, say 1/2, of the fuel. The distance from the shock to the point where the fuel is essentially entirely consumed is also known as the *Zel'dovich–von Neumann–Doering (ZND) length*, L_{ZND}. A 1D detonation in which the extent of the shock plus burning front L_{ZND}, is negligibly small compared to other length scales is a ZND detonation.

One of the major uncertain areas in the study of detonations in both terrestrial and astrophysical contexts is the issue of initiation. As discussed in Sect. 19.7, the question of when a spark in a turbulent environment yields a subsonic flame or a detonation is a difficult one.

Detonation Instability

If a detonation is initiated, it can propagate self-consistently through most of a C/O white dwarf of M_{Ch} before the star can expand to lower densities. In 1D calculations, a carbon detonation can propagate to $\rho \gtrsim 10^6\,\mathrm{g\,cm^{-3}}$. If promptly initiated at the onset of dynamical burning in a white dwarf of M_{Ch}, virtually the whole white dwarf would burn at relatively high densities and thus be converted to iron group elements. This is the basis of the statement that if central detonation is initiated it produces too much iron-group matter.

Two-dimensional calculations of the detonation instability and the resulting cell structure at densities from 1×10^6 to $3\times10^7\,\mathrm{g\,cm^{-3}}$, the range over which detonations are expected to be initiated and to propagate in the context of SN Ia, showed the characteristics expected of detonation instabilities: triple points, transverse waves, weak shocks linking approaching points with each other, and Mach stems connecting the points of reflected transverse shocks with each other and connecting the point of intersection with the boundary (Gamezo et al. 1999; Fig. 19.6). The detonation cell structure grows from initial perturbations and does not depend on those perturbations.

The result is a *pathological detonation* with front speed $S_p > S_{CJD}$ and $Q_p > Q_{CJD}$, where Q_p and Q_{CJD} are the energy released in the pathological detonation and in the corresponding CJ detonation, respectively. In the pathological detonation, the velocity of the front depends on time-dependent details of the reaction kinetics. The computed cell sizes are about 30, 10, and 100 half-reaction lengths for carbon, oxygen, and silicon, respectively.