

1 Overview

1.1 Purpose

The sole purpose of combustion in a reciprocating piston engine is to shift the expansion process away from the compression process in order to generate a working cycle. The only reason for the use of fuel is to generate pressure in order to accomplish this task. This is accomplished by an exothermic (one associated with acquisition of internal energy) chemical reaction, as a consequence of which a transformation (metamorphosis) takes place in engine cylinder between the reactants at initial state, i , attained at the end of the process of compression, and the products at final state, f , established at the start of the process of expansion, as depicted on the pressure-volume (indicator) diagram in Fig. 1.1.

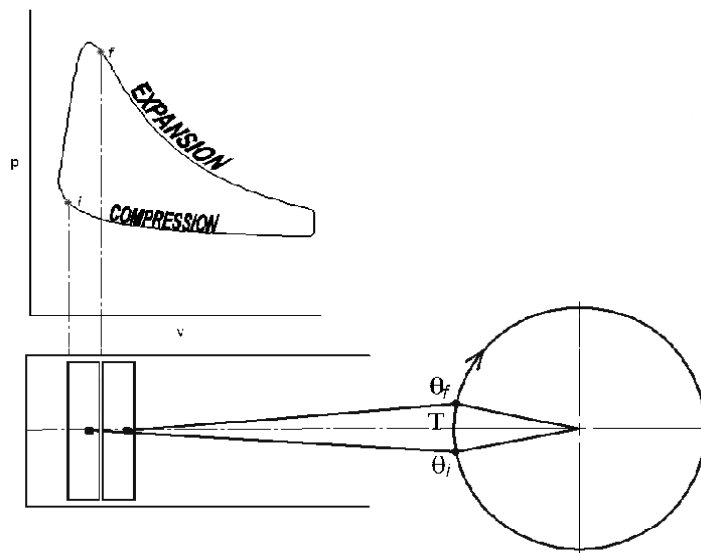


Fig. 1.1. Effective role of combustion in a reciprocating piston engine.
The dynamic stage from i to f , and its lifetime $T = \Theta_f - \Theta_i$.

The directly evident outcome of this process, manifested by the measured pressure data, is referred to as the dynamic stage of combustion. Its lifetime, $T = \Theta_f - \Theta_i$, depicted on the crankshaft circle, is about 1/10 of a rotation. At a maximum speed of 6000 rpm, it is 1 millisecond in duration. At a cruising speed of 2000 rpm it is 3 milliseconds.

So, the fuel, with all the technological, industrial, economic, political and social aspects involved in its supply, accomplishes its effective action in a couple of milliseconds, faster than a blink of the eye – an essential moment of truth. It is also in the course of this short life of the dynamic stage that all the pollutants are formed. What happens there and then is thus of crucial importance to the operation of a piston engine. Described here are some of the fundamental features of this event.

1.2 Combustion

Combustion – the exothermic process associated with oxidation of a hydrocarbon fuel - is the oldest technology of mankind. Over the years this led to a paradox. On one hand, combustion is approached with great reverence, like religion that has to be believed in without understanding. On the other hand, however, it is taken for granted as a consequence of intimate familiarity. The consequences of this paradox cannot be appreciated without some knowledge of this subject. Provided here, therefore, is a concise résumé of what combustion is about and how can it be best utilized in a piston engine.

1.2.1 Reactants

The process of combustion is executed by oxidation of fuel, accomplished by its chemical reaction with air. Fuel is a liquid or gaseous substance consisting of hydrocarbon molecules. A molecule is a bunch of atoms tied together by orbiting electrons.

There are four atoms of major relevance to combustion: carbon, denoted by C, and hydrogen, H, in the fuel; oxygen, O, and nitrogen, N, in air. The chemical expression for a hydrocarbon molecule is C_nH_m , where n and m denote, respectively, the number of atoms of carbon and hydrogen that make it up. For a molecule of octane, for example, $n = 8$, while $m = 18$. Air is predominantly a mixture of oxygen molecules with nitrogen molecules, expressed, respectively by O_2 and N_2 , each consisting, evidently, of two atoms.

1.2.2 Pyrolysis and Dissociation

The chemical reaction of combustion is carried out in two main stages (1) molecular fission and (2) molecular transformation (metamorphosis). First, when heated up, the hydrocarbon molecules become agitated (activated). In an engine cylinder, this is executed either by an electric spark, or by compression. Powerplants utilizing the former are referred to as spark ignition engines, while those using the latter are diesel engines. As a consequence of the agitation, heavy hydrocarbon molecules lose hold of a hydrogen atom and break into lighter fractions referred to as radicals – an action called pyrolysis. As a consequence, the molecules get transformed into hydrocarbon radicals immersed in a “soup” of hydrogen atoms. Relatively light radicals can acquire thereby enough kinetic energy to become *active* in assisting further propagation of the process. Concomitantly, as a consequence of thermal heating, other molecules, such as oxygen, get also split into fractions – an action called dissociation. The processes of dissociation and pyrolysis occur at a temperature level $< 1000 \text{ K}^1$.

1.2.3 Autocatalysis

Thereupon, the hydrogen atom, H – by far the lightest of all the atoms, and hence, the most agitated, the most mobile, the most ubiquitous – ushers in a chain reaction mechanism, playing thus a role of the most effective chain carrier among all other active radicals participating in this mechanism. By hitting (colliding with) an oxygen molecule, O_2 , it gets an oxygen atom, O, split out, while combining itself with the other oxygen atom to form OH – a radical known as a hydroxyl. This event is described algebraically as $\underline{\text{H}} + \text{O}_2 = \text{O} + \underline{\text{OH}}$, where symbols of active radicals are underlined. The oxygen atom, O, as well as the hydroxyl radical, OH, although, respectively, sixteen and seventeen times heavier than the hydrogen atom, play, nonetheless, roles of active radicals by getting involved in propagating the reaction further.

Thus, it is by such a chain reaction mechanism that the molecular transformation is accomplished. Each of the molecular collisions, of which it is made out, is an elementary step. The immediate consequences of initial agitation, such as pyrolysis and dissociation, are the initiation steps. The collisions of one chain carrier generating two chain carriers, as that of a hydrogen atom with an oxygen molecule illustrated above, is a chain branching step. Its threshold temperature is at a level of 1000 K.

¹ Kelvin, an absolute centigrade scale

Ushered in then are propagation steps, where a radical hits a molecule, combines with it, and causes another radical to split off. Eventually, the chain reaction mechanism of hydrocarbon oxidation ends with termination steps, associated with generation of oxygen-saturated molecules: carbon dioxide and hydrogen oxide (water).

The concept of chain reaction mechanism was formulated by Nikolai Nikolaievich Semenov, Nobel Prize Laureate and Director of the Institute of Chemical Physics in Moscow. It was conceived in the study of combustion upon the recognition that it is, in effect, auto catalytic in nature, providing thus the fundamental basis for the catalytic industry. He liked to refer to chain branching as an avalanche. In his eighties, he instituted a program of R&D, in association with automotive industry, to implement the chain reaction mechanism in an internal combustion engine. Its outcome was the so-called LAG² engine, featuring turbulent jet ignition, which attracted a good deal of attention among the automotive community in early 1980's.

1.2.4 Exothermicity

The oxygenated carbon and hydrogen molecules coming out of all these collisions at high velocities behave like a stack of billiard balls hit by a queue ball. Moreover they are rotating and vibrating. The molecules set into these mechanical motions acquire kinetic energies of three kinds: translational, rotational and vibrational. The sum of these energies is expressed as internal energy. The molecules, endowed with this energy, exhibit their agitated (activated) state by high temperature. A process of generating energized products at high temperature is referred to as exothermic. The site where all this takes place is referred to as an exothermic center.

1.2.5 Nitric Oxide

It is by impact of atoms that the molecules of oxygen and nitrogen get dissociated. At a high temperature (around 2000 K), this process forms nitric oxide, NO, one of the major pollutants. The thermal mechanism of generating NO is straightforward: an oxygen atom, O, hits a nitrogen molecule, N₂, yielding NO and O³, while a nitrogen atom, N, hits an oxygen molecule, O₂, producing NO and O⁴. This mechanism was derived by one of the

² Lavina Aktivatsia Gorenia, i.e. Avalanche Activated Combustion

³ $\underline{\text{O}} + \text{N}_2 = \text{NO} + \underline{\text{N}}$

⁴ $\underline{\text{N}} + \text{O}_2 = \text{NO} + \underline{\text{O}}$

most prominent theoretical physicist in Russia, Yakov Borisovich Zeldovich, when he was a teenager.

1.2.6 Chemical Dynamics

Actually, an atom, unlike a billiard ball, is akin in its structure to a solar system of a star (proton) circumscribed by orbiting planets (electrons). A molecule is akin to a cluster of stars. Molecular collisions are, therefore, events of cataclysmic proportions. Their deterministic study, with a sophisticated theory of orbital dynamics supported by molecular beam experiments, is referred to as chemical dynamics – an eminent branch of science distinguished by a number of Nobel Prize laureates.

1.2.7 Chemical Kinetics

In the course of a single chemical reaction, there are many millions of such cataclysmic events taking place. Under such circumstances, one has to deal with millions of colliding worlds! Their eminently appropriate statistical interpretation is referred to as chemical kinetics. Thus, the science of chemical dynamics provides the fundamental background for the subject of chemical kinetics that treats all the atomic and molecular collisions on the basis of statistically established parameters. Collisions between two molecules are called bi-molecular. Collisions between three molecules are termolecular. The rate at which a chain reaction proceeds depends on the frequency of collisions for an elementary step to occur. The frequency is expressed statistically by probability. The probability of the occurrence of bimolecular collisions is, naturally, much higher than of termolecular collisions. To attain a high temperature, however, termolecular collisions are indispensable, because it is only the third partner that carries the gain in exothermic (elevating the temperature) energy generated by the chemical reaction. Their generation is tantamount to the termination steps. It turns out that the principal step for oxidation of carbon monoxide is a bimolecular collision: $\text{CO} + \underline{\text{OH}} = \text{CO}_2 + \underline{\text{H}}$, which is exceedingly slow. So slow, in fact, that it lags significantly behind the essential events of the exothermic reaction, depriving it of the most effective chain carrier, the hydrogen atom, $\underline{\text{H}}$, that could have a catalytic effect upon its evolution.

1.3 Flames

The course of nature is so universal that its outcome is amazingly similar under a wide variety of seemingly dissimilar circumstances. In particular,

the resemblance of the consequences of chain reaction mechanism to the political events of our times is so uncannily fascinating, that it is utilized here to present the rest of the story. The agitated molecules behave as discontented agitators in a malcontent society. They spread out their agitated state at molecular speeds (about 20 % lower than the local speed of sound) - a process known as diffusion. This action has all the earmarks of shooting in the dark: it is carried out at random. The demonstration that random motion is the essential mechanism of molecular diffusion was cited as one of the accomplishments in the certificate of the Nobel Prize for Einstein. It is by this type of communication links that agitators form gangs, where the intensity of agitation can be made so cohesive and effective as to terrorize the rest of the world. In a combustion system left to itself, such as well organized gangs are flames – a set of exothermic centers tied together by molecular diffusion. Flames establish themselves in the form of thin sheets, across which the reactants are transformed (converted) rapidly into products. Their fronts are closed (continuous), delineating contours of the highest temperatures (degrees of agitation) achievable in the combustion field.

1.3.1 Pollutant Formation

A high intensity of agitation is sustained by a tight concentration of exothermic centers. As a consequence of the strong cohesion established by diffusion, once they are formed, it is practically impossible to break them apart. Thus, on one hand, flames are invariably formed when the process of combustion is left to itself to occur naturally, whereas, on the other hand, they maximize automatically the production of all the pollutants. This is so for the following reasons.

The exceedingly high temperature they achieve promotes the formation of nitric oxide. The flame fronts, where the action is, are so thin, that they cannot accomplish satisfactorily their mission of converting the reactants into products. It is for that reason that molecules of carbon monoxide, CO, are left out. Their oxidation into carbon dioxide, CO₂, is so slow that in a well-ordered flame known as laminar, it takes place well behind the front. As a consequence of this delay, the reaction is deprived of the most effective and, hence, the most valuable chain carrier, the hydrogen atom. To make matters worse, the cohesive flame fronts, established behind their diffusion layers, cannot penetrate all the nooks and crannies (cavities) of the cylinder-piston enclosure leaving a good chunk of hydrocarbon fuel completely unprocessed, the reason for an objectionable concentration of unburned fuel in exhaust gases.

Thus, flames are sources of all evil insofar as pollutant formation is concerned. Anything done to inhibit their establishment should go a long way in recovering from the drawbacks of pollutant formation and ineffective fuel utilization, as implied below and elucidated in Part 2.

1.3.2 Pollutant Abatement

It is the intimate familiarity with this essential nature of combustion that led to the concept of external treatment, associated with the technology of chemical processing plants in the exhaust pipe, like catalytic converters. Under influence of a moderately elevated temperature, a catalytic surface in these reactors, be it platinum or palladium, is a donor of oxygen atoms. As one of the chain carriers, this atom provides service in augmenting the rate of oxidation, accomplishing thus the mission of a catalytic agent. But the hydrogen atom does this significantly better and faster in the course of combustion in the cylinder. It acts then, *de facto*, as a catalytic agent, for, as pointed out in the previous section, combustion reaction is intrinsically auto catalytic. Since hydrogen atoms, generated in the course of interior treatment, are much more effective than oxygen atoms provided by surface catalysis of external treatment, the former is fundamentally superior to the latter.

1.4 Knock

The phenomenon of knock played a crucial role in the evolution of the technology of combustion in piston engines. In the past, it was, therefore, of central significance to both, the auto- and the oil-industries. Today, its solution is well known to any motorist in terms of the octane rating of gasoline displayed at all service stations. A similar criterion, in terms of the cetane number, applies to diesel oil. The fact that this is associated with a significant increase in the cost of fuel is accepted as a *fait accompli*.

Upon significant research studies, carried out to explore the physics of detonation phenomena and explosions, it has been established that knock is, in effect, a blast wave⁵ generated by a concentrated deposition of energy in a gas at a high rate. When its shock front interacts with the piston face, it acquires the action of a chisel that hits it, inflicting structural damage, rather than exerting pressure to push. The principal way to advance the technology of combustion in piston engines, advocated here, is associated

⁵ Transient flow field emanating from source at, or around, the center and bounded by a shock front at its periphery

intimately with dilution attained by mixing fuel with extra air, as well as with recirculated residual or exhaust gas. Thus, the localized rate of energy deposition (power density) is concomitantly reduced to such an extent that the onset of knock is annihilated. The octane rating of gasoline can be thereby eliminated – an achievement that can yield an appreciable reduction in the production cost of fuel.

1.5 Prospects

In real life, correcting a misfortune is very difficult, if not entirely impossible. The same applies to combustion. As pointed out above, once a flame is established, it is practically impossible to break it, as long as the reactants are available. In a piston engine, however, one has a multiple sequence of lives. For a car traveling at an average speed, thousands of reincarnations take place per minute. With assistance of modern computer and control technology, any mishap can be, therefore, prevented from occurring again within the time interval of tens of milliseconds available between these reincarnations.

As it should be apparent by now, the main sources of evil are flames, where the exothermic centers are ganged together to form a highly agitated front. This concentrated action is depicted in Fig. 1.2, where the Cal Bears, representing exothermic centers, are forced to cultivate a field by getting bunched together in an overcrowded row at the front.

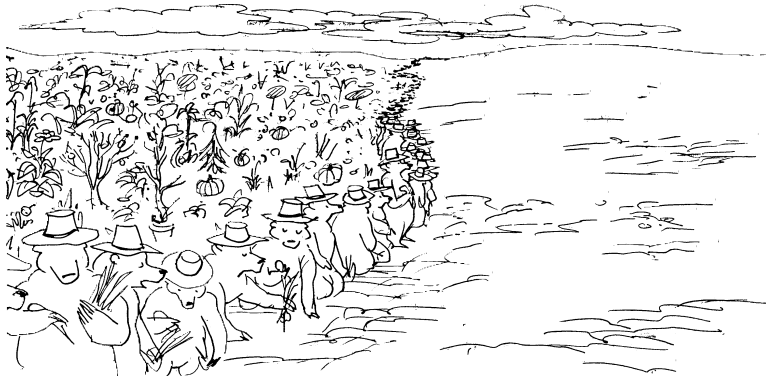


Fig. 1.2. A propagating flame front illustrated by a row of a gang of morose Cal Bears forced to cultivate a barren field in a tight line; drawn by Jean Pierre Petit*

* <www.jp-petit.com>



Fig. 1.3. Distributed reaction centers illustrated by happy Cal Bears, each content to work on his own, while the field is cultivated throughout its full extent, demonstrating the advantage of action in parallel rather than in series. Drawing of Jean Pierre Petit, with portraits of his favorite characters, Monsieur Anselme Lanturlu and his girlfriend, Sofie, with their two wisecracking birds providing voluble comments on what's going on

An alternative way to accomplish the task is illustrated by Fig. 1.3, where the Cal Bears are distributed, each having fun in cultivating his individual flowerpot. The cultivation, performed painstakingly in series by a propagating front of malcontent bears, is accomplished in parallel much better and faster when they are happy for being treated as well as they ought to be. Therefore, instead of permitting flames to be established beyond any control, one should not let exothermic centers to agglomerate into delinquent gang-lines.

In an engine cylinder adequate distribution of exothermic centers to prevent the formation of flames can be attained by dilution. This can be accomplished either by pre-mixing fuel and air using RGR⁶ or EGR⁷, or injecting turbulent jets of super-rich air/fuel mixture into a piston-compressed air combined with a certain amount of RGR or EGR. The concept of premixing the combustible charge with a relatively large amount of residual gases gained today quite a lot of popularity under the name of HCCI⁸. The adjective "Homogeneous" implies in reality the distribution of exothermic centers portrayed by Fig. 1.3, whereas "Compression Ignition" is handicapped by uncontrollability. However, dilution of the charge offers remarkable means to inhibit the occurrence of knock as a consequence of the diminished concentration and amplitude of exothermic centers, reflected by a decrease in local exothermic power density.

⁶ Residual Gas Recirculation

⁷ Exhaust Gas Recirculation

⁸ Homogeneous Charge Compression Ignition

It is quite reasonable to expect that the execution of the exothermic process could be monitored and modulated for this purpose by a micro-electronic control system of a CCE⁹. Conceptually, the electronic apparatus consisting of micro-sensors for monitoring pressure and MEMS¹⁰-type devices for operating its micro-valves could be accommodated within a 'smart cylinder head' that, eventually, may be miniaturized to a "smart cylinder gasket". The control system will be governed by a microprocessor. As pointed out above, its task will have to be accomplished for each combustion event within a time interval of an order of a millisecond between two consecutive cycles – well within the capability of modern electronics.

To sum up, the secret of success in controlling combustion is based on the political adage of Julius Caesar: DIVIDE ET IMPERA.

⁹ Controlled Combustion Engine

¹⁰ Micro-Electro-Mechanical-Systems