Introduction to Physics and Chemistry of Combustion

Explosion, Flame, Detonation

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Combustion is a truly interdisciplinary subject, and as such it requires merging of different areas of science: hydrodynamics, chemical kinetic, thermodynamics, statistical physics, kinetic theory, and quantum theory. Due to such a complexity the in-depth scientific investigation of combustion is a recent phenomenon, even though it has always had a great impact on all types of human activities. The elements of combustion, such as flame and explosion are, of course, known for a long time but somewhat surprisingly their first analytical description has been obtained not such a long time ago and for only a limited range of conditions. A more coherent picture has begun to emerge in recent times, as a result of a number of experimental and theoretical studies, sponsored by energy production and industrial needs.

Combustion has a wide variety of uses. Chemical combustion is used for energy’s production in power plants, gas turbines and engines. Similar process of thermonuclear combustion is a heat source for the Sun and stars. Recently, astronomers were using exploding stars known as Type Ia supernovas as a cosmic standard light markers to analyze the fate of the universe. They found that the universe expansion is speeding up rather than slowing down, whereas previously it was expected that gravity would be slowing down the expansion. Combustion is involved in explosions for both industrial and military purposes. The humanity cannot live without combustion processes but they also have harmful effects, such as unwanted fire and explosions, pollutants and greenhouse gases, which cause global warming.

Combustion is a process of heat release in exothermal reactions, which is accompanied by mass and heat transfer. The chemical combustion involves a chemical transformation between a substance or substances called fuels and other chemicals called oxidizers. In the process, nuclei of the entering substances are not altered but bonds, involving the electrons of the molecules and atoms, are changed. In many cases, it leads to heat being released, while other cases, heat is required to form the bonds. Heat release in the process of bonding change is the most interesting since this energy can be captured and usefully exploited. Combustion may involve all phases of matter – solid, liquid and gas: solid rocket propellants, liquid droplets burning in diesels, and gaseous combustion in SI-engines. The principal difficulties in understanding combustion
systems are the wide range of time and space scales involved, chemical complexity and multidimensional nature of the flow configuration. In turbulent combustion, the strong non-linear coupling of the turbulence and the chemistry further compounds difficulties. These turbulence-chemistry interactions arise from the fact that in most combustion systems, mixing processes are not fast compared with rates of chemical reaction, and there are large spatial and temporal variations in species’ composition and temperatures. Chemical reaction’s rates are strongly coupled to molecular diffusion at the smallest scales of the turbulence. Furthermore, the heat release associated with combustion affects the turbulent flow, both from variations in the mean density field and from the effects of local dilatation. In the face of such difficulties for a direct analytical approach, engineers have traditionally resorted to empirical methods to develop a combustor. While in the last century the empirical approach sufficed, today there is a much stricter control of pollutant emission and a need for a much more effective burning of fuel, which makes empirical approach no longer viable.

Most of the material covered in this book will deal with the gas phase and with premixed gas combustion. Premixed gas combustion is combustion of gaseous reactants, perfectly premixed prior to ignition. In that case, one has only to ignite the mixture in order to initiate a reaction. The most distinctive feature of premixed combustion is its ability to form a self-sustained reaction wave propagating with a well defined speed, which is either larger (detonation wave) or much less (deflagration wave, “flame”) than sound velocity. Thus, we can say that these two regimes of reaction wave, deflagration and detonation, appear to be stable attractors each being linked to its own base of initial data. Premixed gas combustion is obviously of utmost practical importance in engines, modern gas turbines and explosions. There the fuel and air are premixed, and combustion occurs by the propagation of a front separating unburned mixture from fully burned mixture. The emphasis in the present course will be placed on regimes of premixed combustion due to its key importance for practical applications.

While there are several outstanding combustion text-books, they are too advanced and may be difficult for introducing the subject at the undergraduate level. These texts are primarily aimed at the audience at a more advanced level. The present book is primarily meant for 2nd and 3rd year university students, and for PhD students working in the field of physics, chemistry, mechanical engineering, computer science, mathematics and astrophysics. However, many researchers who already work in the combustion will find some useful background material as well as an overview of recent major developments in this field. This book has been developed through modification of my lecture notes of the combustion course that I have taught for the last several years. The book is focused mainly on theoretical modeling and fundamentals of physics and chemistry of combustion processes and on physics mechanisms for various combustion and combustion-related phenomena in gaseous combustible mixture. The combustion of a gas mixture (flame, explosion, detonation) is
necessarily accompanied by motion of the gas. The process of combustion is therefore not only a chemical phenomenon but involves the study of gas dynamics. Therefore, we have included elements of fluid dynamics, which are usually missing from university courses. While assuming that first year physics, chemistry, calculus and thermodynamics have been taken, the necessary concepts in thermodynamics and fluid mechanics are presented during the course.

A vast number of combustion research has been published in multi-disciplinary scientific journals, such as Physical Review as well as in specialized combustion journals, such as Combustion and Flame, Combustion Theory and Modeling, Combustion Science and Technology, Journal of Fluid Mechanics, etc., as well as many volumes of Proceedings of Combustion Institute (International), so that a list of references would consist of thousands of studies. Instead of giving a list of enormous number of references, I offer a short list of books for further study for an interested reader.


I want to thank many of my colleagues and PhD students whose interest in and devotion to the combustion research have enormously helped in forming the newer concepts of combustion wave and assisted with the illustrations used in the book. I am gratefully acknowledge help and discussions with A. Ivanov and M. Kuznetsov of the problem of deflagration-to-detonation transition, and M. Kuznetsov and I. Matsukov providing me with their valuable experimental data of deflagration-to-detonation transition.

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Sources and Use of Energy

Today’s world energy consumption is about 1 Q/year with annual growth of about 5%. The unit Q, which is used for such large amounts of energy, roughly equals to $1.05 \cdot 10^{21}$ J. This is a huge amount of energy, which is enough to vaporize approximately 4 trillion of cubic meters of water, the amount of a very large lake. Solar radiation annually absorbed by the Earth is approximately 15,000 Q. To avoid drastic change of climate the energy input produced additionally by human activity must be limited to about 0.1% of this value. This means that upper limit for energy annually produced by human activity should not exceed approximately 15 Q. With the present increase of energy consumption we shall have reached this limit in about 30–40 years. Yet a more serious problem is pollutant emission caused by combustion. Today world energy production is dominated by carbon-based fuels, such as oil, natural gas and coal and hence combustion provides over 85% of the total energy. As such, it is also the principal contributor to air pollution.

It is unlikely that by the end of the twenty-first century other energy sources will have become serious competitors to hydrocarbon combustion. Nuclear energy has a limited appeal because of prejudice and, in some cases, political reasons, and so it will probably not become a significant source of energy. Improved breeder nuclear reactors would be able to provide a temporary relief for the energy problem but this would also mean an easier unauthorized access to the weapon-grade nuclear materials. The reserves of nuclear fuel are limited, even compared to coal. Perspectives for thermonuclear energy production remain uncertain. Up-to-date progress in controlled fusion research has turned out to be much more modest than was expected earlier, in the 1960s. One does not presently expect that the controlled fusion becomes an industrial energy source before the end of the century. The solar energy’s use requires huge investments, in particular, for producing new materials allowing a substantial reduction in solar energy costs. Additionally, solar energy production is a viable option in a relatively limited geographic area, mainly outside of the developed countries, and hence relying on it would make developed countries dependent on the political stability of those potential solar energy providers. Even then, countries, which are enjoying a lot of sunshine, still do not have particular encouraging prospects for solar energy.
It has been anticipated that fuel cell systems will play an increasing role in power generation, reducing green house gases' emissions and slowing the global warming. In general, vehicles and power plants, which would use stored hydrogen as fuel, could ultimately reduce local petroleum consumption and local air pollution. However, to achieve this goal one requires a practical, economical hydrogen source that does not generate carbon dioxide. The development of such a hydrogen source, as well as hydrogen’s storage and distribution, present a major challenge for fuel-cell technology. At present, producing hydrogen by electrolysis would require to double the total generation of electrical energy to power cars by fuel-cells. Much more energy is needed to produce a quantity of hydrogen compared to the energy than can be obtained from it by combustion or by reactions in a fuel cell. Indeed, energy required is the difference between the heat of combustion of the resulting hydrogen and the heat of combustion of the reformed feedback. This difference sets the lower limit on the energy required to produce an alternative fuel. In practice, the overall efficiency of the process – that is, the energy content of the hydrogen produced divided by the total energy consumed by the reforming process is less than 60%. This means that to produce an amount of hydrogen with the energy content 1 MJ, we must spend more than 1.6 MJ of energy. But, only 0.167 MJ must be expanded to produce a quantity of gasoline with energy content of 1 MJ. Thus, use of hydrogen produced by reformation does not free us from dependence on hydrocarbons. Since nuclear power and renewable energy sources, such as hydropower, solar and wind, are not expected to expand enough to support the electrolysis of seawater, the only realistic source for hydrogen fuel is through reforming of petroleum or natural gas. The process of extracting hydrogen from fossil hydrocarbons using very hot steam, for example, will produce as much carbon dioxide as if the fuel had been burned conventionally. If that CO₂ is not sequestered by some means, preferably near the hydrogen plant, its release into the atmosphere will cause as much global warming as if it had come from conventional car or thermal power plant.

Recent climate catastrophes such as hurricanes Katrina and Rita, which hit New Orleans, Texas and Florida, as well as storms and floods in Asia and Europe, all present us with a serious warning of the climate change, caused by the global warming due to release of pollutants into the atmosphere. The main danger for societies and their economies is not a shortage of oil and gas and resulting rise in prices of hydrocarbon fuels but rather the global warming. It is generally accepted that burning of the hydrocarbon fuel, which is vitally necessary for industry and transportation, is the main source of the pollutants, which are causing global warming. Combustion is responsible for nearly all of the emission of NOₓ, CO, CO₂, aerosols, and many other chemical species that are harmful to human health and the environment. According to the environmentalists, the first and most reliable signs of an impeding climate catastrophe are the upsurge in the most violent storms. There is a sustained increase in the number and intensity of catastrophic storms over the last 30 years. Carbon dioxide and other greenhouse gases produced in combustion
elevate the atmospheric temperatures causing global warming. As a result, when ocean temperature rises, the amount of water vapor in atmosphere will rise as well. A moister atmosphere helps fuel storms as they have more to “spit out” in form of rain and also by helping drive the convection that gives them lethal spin.

Typical combustion processes are inherently multi-scale, involving complex spatio-temporal phenomena, associated with chemical reactions, molecular transport, and turbulence. The considerable disparity between various scales poses formidable difficulties both for theoretical analysis and numerical simulations, and their effective resolution is one of the main issues of the combustion research. Nowadays science and engineering have reached the point where the ability to simulate processes at very small scales of space and time is essential for furthering our understanding of the whole processes. The ability to simulate processes involving a wide range of spatio-temporal scales and adequate chemical kinetics is essential for furthering understanding of burning processes and for developing the tools required for development of new energy technologies. This understanding is crucial for realizing the long-term goal of creating an environmentally and economically sustainable energy source. The anticipated advances in computational power together with theoretical combustion models offer an opportunity to revolutionize the design and performance of combustion systems, which will considerably lower emissions and increase thermodynamic efficiency of new combustion technologies.

In conclusion, we will give some representative numbers of the world reserves of hydrocarbon fuels and their distribution. The world reserves of coals is 144 Q; of oil, 7–8 Q; of natural gas, 1–2 Q. With the present level of consumption, the reserves of oil and gas will have been depleted in 50 years. All reserves of hydrocarbon fuels may be exhausted in about 100 years, although neither the exact energy needs nor the precise reserves are known with the accuracy which is needed to make definitive predictions.
Chapter 1
Basic Concepts of Thermodynamics

Combustion is one of the most complex subjects that involve primarily such disciplines as physics, chemistry, thermodynamics and fluid mechanics. Thermodynamics enables us to calculate the energies of system changes in composition. As such it enables us to determine, for example, the temperature and pressure changes when a system undergoes a chemical transformation. It will be seen that thermodynamics can also be used to tell us what the composition change will be when a system undergoes a reaction. It is not used however to determine rates of chemical transition. That is the subject of chemical kinetics. The subject of thermodynamics is only concerned with beginning and end thermodynamic states for a system, with no concern for the process path between them. Therefore it will be important to recall the necessary basic concepts of thermodynamics in this course. The purpose of this chapter is to make students life easier, by providing review of the main basic concepts of thermodynamics and necessary definitions. Similarly, in several chapters below the necessary concepts of fluid mechanics will be given, some of them usually missed in standard courses of fluid mechanics.

1.1 The Entropy

Thermodynamic physical quantities are those, which describe macroscopic states of system. They include some, which have both a thermodynamic and a purely mechanical meaning, such as energy, volume, density, etc. There are also, however, quantities of another kind, which appear as a result of purely statistical laws and have no meaning when applied to non-macroscopic systems, for example, entropy. In what follows we shall define a number of relations between thermodynamic quantities. When thermodynamic quantities are discussed, the negligibly small fluctuations to which they are subject are usually of no interest, so that, we shall entirely ignore such fluctuations, regarding the thermodynamic quantities as varying only with the macroscopic state of the system.