

**FLAME, DETONATION, EXPLOSION –
WHEN, WHERE AND HOW THEY OCCUR**
(plenary lecture)

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ABSTRACT

Combustion is also involved in explosions for both peaceful and military purposes. In the past decades, there has been a considerable progress in understanding combustion processes and regimes of the combustion propagation. This review focuses solely on explaining various phenomena of premixed combustion: (1) flame propagation, (2) detonation waves, (3) when and how explosions occur, (4) the transition from flame to detonation and (5) when ignition of combustion involves phases of deflagration or detonation. Additionally, the paper will include a discussion of what pollutants are produced during combustion and how clean and efficient combustion can be achieved. Examples of typical combustion scenarios, including flames propagating in tubes, closed chambers or engines are overviewed, along with events of the thermonuclear Supernova.

Results obtained during past decades on the dynamics of flames, the understanding of the nature of burning and mathematical descriptions and numerical modelling of combustion are outlined. I shall talk about such prominent scientists as Yakob Zel'dovich and Lev Landau who were at the origin of modern combustion theory and made fundamental contributions to the understanding of combustion.

1. INTRODUCTION

Combustion is a subject, which is truly interdisciplinary requiring the merging of knowledge in different subjects of physics and chemistry, including hydrodynamics, chemical kinetic, thermodynamics, statistical physics, kinetic theory, and quantum theory. That's why although combustion has a very long story, which is comparable with the time of human story (we can count at least from the Prometheus time) and great economic and technical impact on almost all sides of human activity, its scientific investigation is of relatively recent origin.

Combustion has a wide variety of uses. Chemical combustion is used for energy production in power plants, gas turbines and engines. Similar process of thermonuclear combustion is a heat source in the Sun and stars. Combustion is also involved in explosions for both industrial and military purposes. Though people are beneficial from using combustion, it however has harmful effects such as unwanted fire, explosions and pollutants and greenhouse effects are produced. Combustion is a process of heat release in exothermal reactions, which accompanied by mass and heat transfer. Combustion can involve all phases of matter – solid, liquid and gas, for example, in solid rocket propellants, liquid droplets burning in diesels, and gaseous combustion in Otto engines.

List of the names of people who made notable contributions in foundation of the combustion science is too long to be given here. These are names of Lavoisier, Bunsen, Le Chatelier, Chapman, Jouguet, and many others. I would like to mention names of a great physicists from Russia – Yakov Zel'dovich and Lev Landau, whom I new personally. Virtually all aspects of modern combustion theory bear marks of the names Landau and Zel'dovich. There are many good combustion textbooks, which are aimed at a wide audience from graduate students to scientific researchers and engineers. One of these books written by prominent researchers A. Linan (Spain) and Williams (USA) starts by the following dedication: "To Ya. B. Zel'dovich Who erected the Foundation of the Modern Science of Combustion."

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 difficulties are further compounded by the complexities of chemical kinetics and the strong non-linear coupling of the turbulence and the chemistry. 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 large spatial and temporal variations in species composition and temperature are present. Chemical reaction 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, engineering practice has traditionally resorted to empirical methods for combustor development. While in the last century empirical methods were sufficient for development of combustors, today the market place demands much stricter control of pollutant emission and much more effective burning of fuel.

Regimes of combustion and flame dynamics will be of the first priority in this review and we shall not go into details of chemical aspects of the burning process. Realistic burning in a flame may involve up to thousands elementary reactions. Still for a simple estimate most of details of chemical reactions are not important so that some combustion features may be described satisfactory by use of highly idealized model of one simplified irreversible reaction that transfer the fresh fuel mixture into the products of burning. We will also consider here premixed gas combustion, which is the opposite case to diffusion flames. Premixed gas combustion is the combustion of gaseous reactants, which are perfectly premixed prior to

ignition. This implies that all components necessary for the reaction are present in the fuel mixture from the very beginning and in order to initiate reaction one has only to ignite the mixture. Premixed combustion is of practical importance in engines, modern gas turbine and explosions, where the fuel and air are essentially premixed, and combustion occurs by the propagation of a front separating unburned mixture from fully burned mixture. Since premixed combustion is the most fundamental and potential for practical applications, the emphasis will be placed on regimes of premixed combustion and numerical methods for solving the corresponding transport equations.

2. REGIMES OF REACTION WAVES PROPAGATION

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 or much less than sound velocity. A remarkable feature of premixed combustion is a strong dependence of the chemical reaction rate on temperature expressed by the Arrhenius law for the reaction rate $k = A \exp(-E/RT)$, where E is the activation energy. The activation energy of many reactions is so large, that the reaction rate at the room temperature may be taken zero. On the contrary, increase of the fuel temperature even by a factor 2-3 may lead to the increase of the reaction rate by many orders of magnitude and to a noticeable reaction (Zeldovich et al. 1985). In the case of a strongly exothermic reaction when a considerable energy release is involved, relatively slight increase of the temperature at some region ignites the reaction, which eventually extends over the whole gas.

Two main regimes of combustion should be distinguished: strongly subsonic regime, which is known as a flame, or deflagration, and supersonic regime of the reaction wave propagation known as detonation. In the case of a flame the physical mechanism of flame propagation may be described as follows. The burnt matter has larger temperature and thermal conduction transports energy from the hot burnt matter to the cold fuel. The temperature of the fuel close to the burnt matter increases, the reaction in this fuel goes faster until another portion of the fuel is burnt and some additional energy is released. The released energy is transported by thermal conduction to the next fuel layer resulting in propagation of the reaction front. Thus, a flame or *deflagration* is the combustion regime, which is due to heat diffusion – the direct transfer of heat from the burning gas to the fresh fuel, which is still unburned.

Flame velocity and thickness of a flame front may be estimated on the basis of a simple dimensional analysis (Landau and Lifshitz, 1987). If the burning process is characterized by the typical time τ_b , then the only combination of velocity dimension that may be constructed out of the thermal diffusivity $\kappa / \rho_f C_p$ and the reaction time τ_b is

$$U_f \propto \sqrt{\frac{\kappa}{\rho_f C_p \tau_b}}, \quad (1)$$

where κ is the coefficient of thermal conduction and C_p is the specific heat of the fuel at constant pressure and ρ_f is the gas (fuel) density. Obvious conclusion from the estimate Eq. (1) is that the smaller the reaction time and the stronger the thermal conduction, the faster flame propagates. Acting in a similar way, we can obtain expression for the flame thickness

$$L_f \propto \sqrt{\frac{\kappa \tau_b}{\rho_f C_p}}, \text{ or being expressed in term of the flame velocity}$$

$$L_f = \frac{\kappa}{\rho_f C_p U_f} \quad (2)$$

The equations (1) and (2) are a simple dimensional consequences of the equation of thermal conduction.

If we use the estimate for thermal diffusivity coefficient expressed through the sound speed c_s and the mean free time τ_{coll} : $\kappa \rho_f C_p \approx c_s^2 \tau_{coll}$, then we obtain $U_f / c_s \propto \sqrt{\tau_{coll} / \tau_b}$. Since only a very small fraction of colliding molecules participates in chemical reactions because of the large potential barrier of a reaction (because of a large activation energy), so $\tau_{coll} \ll \tau_b$. We come to the conclusion that velocity of flame propagation is much smaller than the sound speed: $U_f \ll c_s$.

Typical velocities of the flame range between 5 cm/s and several meters per second. Flame in the hydrogen-oxygen mixture propagates with the velocity about 9 m/s and it is one of the fastest one, while the flame in the mixture 6% CH₄ and air is one of the slowest ones with the velocity 5 cm/s. Such slow flames are usually close to extinction limits because of some inevitable losses. With representative values for κ , C_p and ρ for gas mixtures we find that the typical thickness of combustion zone ranges from $5 \cdot 10^{-2}$ to $5 \cdot 10^{-4}$ cm.

If we consider another type of a flame instead of chemical one, then the energy release may be supplied from other sources. An example of other energy sources is thermonuclear reactions in Supernova flames (Timmes and Woosley, 1992) or the laser radiation absorbed by plasma layers close to the critical surface of a target in inertial confined fusion (Manheimer et al. 1982). For any kind of flames the released energy is transported by thermal conduction and flame propagates relatively slow compared with the sound speed. This is a subsonic regime of reaction propagation.

Flame is not the only possible self-supporting regime of reaction propagation. A reaction can also propagate in a fast supersonic regime of detonation (Landau and Lifshitz, 1987). In the case of a detonation the reaction is induced by a shock wave compressing and heating the fuel. The burning mixture expands and acts like a piston pushing a leading shock and supporting the detonation. From the technical point of view detonation is a very undesirable process that can damage engines. Transitions from the slow regime of flame propagation to a detonation regime are observed quite often in experiments (Shelkin, 1940, 1966; Zeldovich et al., 1985).

Sometimes a third regime of burning is distinguished, which is the regime of spontaneous reaction (Zeldovich, 1980). A spontaneous reaction corresponds to the configuration of a fuel with a non-uniform initial temperature distribution. In this case subsequent (though independent) development of the reaction in the neighboring fuel layers may be interpreted as propagation of a reaction front with the front velocity depending on the initial temperature distribution. Though the regime of spontaneous reaction is much more specific than the regimes of flame and detonation, it may be also interesting from the point of view of flame/detonation ignition.

3. STRUCTURES OF PREMIXED FLAMES

Structure and propagation velocities of gaseous premixed laminar flames depend on transport properties of the fuel gas and chemical-kinetic rate parameters. Questions of interest include the local structure of the flame front, and the most important - velocity of the flame. Structure and dynamics of a flame is described by the hydrodynamic equations of mass, momentum and energy conservation with the account of reaction kinetics and transport processes of thermal conduction, fuel diffusion and viscosity. If for the sake of simplicity we assume a single irreversible reaction, then the governing equations are the following:

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} (\rho v_i) = 0, \quad (3)$$

$$\frac{\partial}{\partial t} (\rho v_i) + \frac{\partial}{\partial x_j} (\rho v_i v_j + \delta_{ij} P - \tau_{ij}) = \rho g_i, \quad (4)$$

$$\frac{\partial}{\partial t} \left(\rho e + \frac{1}{2} \rho v_i v_i \right) + \frac{\partial}{\partial x_i} \left(\rho v_i h + \frac{1}{2} \rho v_i v_j v_j + q_i - v_j \tau_{ij} \right) = \rho g_i v_i, \quad (5)$$

$$\frac{\partial}{\partial t} (\rho Y) + \frac{\partial}{\partial x_i} \left(\rho v_i Y - \kappa \frac{\text{Le}}{C_p} \frac{\partial Y}{\partial x_i} \right) = - \frac{\rho^n Y^n}{\rho_R^{n-1} \tau_R} \exp\left(-\frac{E}{T}\right), \quad (6)$$

where Y is the fuel mass fraction, $e = QY + C_v T$ is the internal energy, $h = QY + C_p T$ is the enthalpy, C_p and C_v are specific heats per unit mass at constant pressure and volume respectively, their ratio determines the adiabatic exponent $\gamma = C_p / C_v$, \mathbf{g} is a gravitational field. In the development of the reaction the fuel fraction changes from 1 to 0. We consider a reaction of the order n with the energy release Q ; the Arrhenius law gives the temperature dependence of the reaction rate with the activation energy E (taken in temperature units) and with constants of time dimension τ_R and density dimension ρ_R . Usually the reaction order is of no importance for hydrodynamic properties of a flame with the exception of the problem of flame dynamics in a closed burning chamber, where flames with the first, second and third order reactions behave in a different way. The stress tensor and the energy diffusion vector are given by the formulas

$$\tau_{ij} = \kappa \frac{\text{Pr}}{C_p} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right), \quad (7)$$

$$q_i = -\kappa \frac{\partial T}{\partial x_i} - \text{Le} \kappa \frac{Q}{C_p} \frac{\partial Y}{\partial x_i}, \quad (8)$$

where Pr is the Prandtl number characterising the relative strength of viscosity and thermal conduction and Le is the Lewis number that shows the relative role of fuel diffusion and thermal conduction. Generally, the gas mixture can be treated as a perfect gas with the equation of state

$$P = \frac{\gamma - 1}{\gamma} C_p \rho T. \quad (9)$$

The set of equations (3)-(9) is typically used in direct numerical simulations of flame dynamics.

The simplest configuration of a flame is a planar stationary flame. The problem is considerably simplified in the case of a planar stationary flame. In the reference frame of the flame front the flow consists of a uniform flow of the fresh fuel mixture entering the flame front with the velocity $v_z = U_f$, of the region of heating and reaction (which is the flame front itself) and of a uniform flow of the burnt downstream. Then, the structure of the heating and reaction region and the velocity of the planar flame front as a function of the thermal and chemical fuel parameters can be found by solving a stationary version of the equations (3-9) with the boundary conditions in the fuel and in the burnt matter

$$T = T_f \quad \text{for} \quad z = -\infty; \quad T = T_b \quad \text{for} \quad z = \infty. \quad (10)$$

The temperature of the burnt matter depends only on the fuel temperature and the energy release in the reaction and may be expressed through the expansion coefficient as $T_b = \Theta T_f$. Equation (2.21) together with the boundary conditions (2.24) constitute an eigenvalue problem, where the flame velocity U_f is the eigenvalue and the flame internal structure $T = T(z)$ is the eigenfunction.

The Zeldovich - Frank-Kamenetski theory of planar stationary flames takes into account the fact that typically the activation energy of the reaction is very large $E/T > E/T_b \gg 1$. This asymptotic (analytical) theory is in a very good agreement with numerical solution of Eqs. (3-9) (Liberman et al., 1994). Characteristic thickness of the reaction zone L_R where temperature is close to the final value $(T_b - T)/T_b \propto T_b/E$ is much smaller than the total flame thickness $L_R \propto L_f T_b/E \ll L_f$. For the flame thickness we obtain

$$\frac{\kappa_b}{2C_p} \frac{T_f^2 (\Theta - 1)^2}{L_f^2} = \frac{\rho_f T_f}{\tau_R T_b} \frac{T_b^4}{E^2} \exp(-E/T_b). \quad (11)$$

and for the flame velocity

$$U_f = \left(\frac{2\kappa_b}{C_p \rho_f \tau_R} \right)^{1/2} \frac{\sqrt{\Theta} T_b}{\Theta - 1} \frac{1}{E} \exp\left(-\frac{E}{2T_b}\right). \quad (12)$$

These expressions are consistent with the predictions of the dimensional analysis Eqs. (1,2).

Figs. 1(a,b) illustrate schematically the flame structures for premixed flame (1a) and diffusion flame (1b), respectively, calculated with a simplified assumption of one-step Arrhenius chemistry based on activation-energy asymptotic for large Zel'dovich numbers.

4. HYDROGEN, CARBON MONOXIDE, HYDROCARBON PREMIXED FLAMES

The structure of flames is determined by competition between radical formation and radical consumption reactions and differs considerably from the structure obtained from one-step high activation energy models. For example, thickness of the reaction zone obtained from one-step high activation analyses is small compared with the flame thickness derived from the maximum temperature gradient. For real kinetics they are of the same order. Furthermore, at least two chemical time scales are necessary to describe the structure of practical laminar premixed flames: one associated with the chain branching of radical reactions and another associated with the three-body recombination reactions. In industrial applications we deal with situations when the flame front is affected by the turbulence already present in the flow or generated by the combustion process.

Abilities to describe all types of data have progressed during the past years; most notably, there has been remarkable progress in determining chemical-kinetic rate parameters. Nevertheless, it needs to be borne in mind that typical uncertainties in values of high-temperature transport properties are on the order of 10% or more and generate uncertainties of about this same order in computed flame structures. The major barrier, however, is the much larger uncertainties in chemical-kinetic parameters, combined with difficulties in computing flame structures with detailed chemistry. Flame-structure calculations with detailed chemistry used to be arduous tasks pursued by only a few devoted experts. Most rate parameters of combustion chemistry used to be deduced from fits to overall measured combustion properties, leading to large uncertainties, often exceeding an order of magnitude, because of

interdependencies of various unknown rates, for example. Presently the rate of the single most important elementary reaction in combustion, the branching step $\text{H} + \text{O}_2 \Rightarrow \text{OH} + \text{O}$; is known to be better than 5% over the temperature range of interest in combustion. Current direct numerical simulation for turbulent premixed flames is mainly for one-step high-activation energy kinetics for 3D modeling or employs more or less realistic kinetics for 2D simulations.

Hydrogen-air flames are special in that no more than about 20 elementary reactions are relevant to their primary chemical kinetics, and the rate parameters for these are known better than those of other flames. There still are uncertainties, such as third-body efficiencies and associated temperature dependences for recombination steps such as $\text{H} + \text{O}_2 + \text{M} \Rightarrow \text{HO}_2 + \text{M}$. Empirical one-step Arrhenius approximations for hydrogen-air flames required comparatively low overall activation energies, and detailed chemistry descriptions is needed.

Systematically reduced chemistry has been studied in efforts to further clarify hydrogen-air flame structure. Systematic reduction of the chemistry is achieved by introducing appropriate steady-state or partial-equilibrium approximations into detailed chemistry and neglecting terms and reactions of lesser importance to achieve simplified descriptions of the flame structure. This kind of approach has been known since the work of N.N. Semenov.

From the viewpoint of reduced chemistry, hydrogen oxygen flames are relatively simple even with no reduction, since they involve only the eight species H_2 , O_2 , H_2O , H , OH , O , HO_2 and H_2O_2 and possess two element conservation equations. The full-chemistry description is only a six-step description, as judged from the viewpoint of the number of overall steps that are derived by reduced chemistry.

Steady-state approximations for the intermediate H_2O_2 , HO_2 , O , OH and H results in five, four, three, two and one-step reduced-chemistry descriptions.

In the one-step description, $2\text{H}_2 + \text{O}_2 \Rightarrow \text{H}_2\text{O}$ proceeds mainly at the rate of the three-body elementary recombination step. This extent of reduction gives a terrible result, while the two-step description

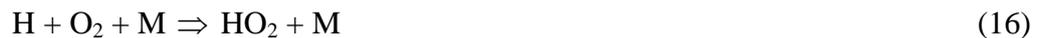


is much better. Here step (13) proceeds mainly at the rate of the aforementioned chain-branching step and step (14) at the rate of the recombination step. Even at this stage, the description is not very accurate, since OH and O do not strongly obey good steady states, but it provides a qualitatively much better description and does contribute significantly to understanding of the flame structure.

The active radical H is needed for flame propagation: the branching rate



that generates radicals increases with temperature, while the recombination rate



is nearly independent of temperature.

The downstream reaction zone where branching occurs can be very broad and extend over most of the temperature range.

This concept of flamelet structure differs from that of one-step activation-energy asymptotics, which can be made to fit the picture only by having a fairly broad reaction zone, thereby requiring rather low activation energy. This explains why one-step Arrhenius approximations need overall activation energies that vary with conditions.

Carbon monoxide flames share a lot in common with hydrogen flames because they generally need the hydrogen oxygen branched chain to propagate.

The methane–air flame is the simplest hydrocarbon flame. The hydrocarbon chemistry, however, consists of much larger the number of elementary steps that must be considered to address its structure with detailed kinetics and substantially increases the number of chemical species involved. Although the most relevant chemical rate parameters are now fairly well known, the situation certainly is not as satisfactory as that for flames of hydrogen or carbon monoxide. The detailed reaction mechanism in current description of the oxidation of n-heptane includes 2450 elementary reactions among 550 chemical species.

In view of the large number of elementary steps, concepts of reduced chemistry is much more helpful for hydrocarbon flames than for hydrogen flames. For methane–air flames, a four-step reduced-chemistry description has been identified, which includes the fuel-consumption step



in addition to steps (13, 14) and the overall step



which is at the rate of the elementary step $\text{CH}_4 + \text{H} \Leftrightarrow \text{CH}_3 + \text{H}_2$.

The fuel chemistry, proceeding through methyl, formaldehyde and formyle, has the net effect of removing radicals, as indicated by step (18). Consequently radicals tend not to exist where there is an appreciable amount of fuel. An effective overall activation energy can be defined and it does depend on rate parameters of elementary steps, but not in a simple way, contrary to the classical one-step Arrhenius description.

5. POLLUTANT PRODUCTION

During the past years, environmental concerns have prompted extensive consideration of emissions of pollutants from flames, leading to clarifications of finer details of flame structures. Different pollutants force focus on different chemistry, since the chemical kinetics is specific to the pollutant. Addressing emissions of oxides of sulfur, for example, therefore leads to consideration of sulfur chemistry. Much of the recent research has been devoted to the formation of polycyclic aromatic hydrocarbons and of oxides of nitrogen, as well as to emissions of soot. It therefore seems convenient to place the work in two broad classes, namely production of larger molecules through fuel chemistry and production of oxides of nitrogen through nitrogen chemistry.

Pollutants derived from fuel chemistry include both PAH species and soot, one of the contributors to emissions of particulate matter. The chemical kinetics of PAH and soot in flames is very complex and involves very large numbers of elementary chemical steps among large numbers of trace species. In addition to these chemical challenges, soot further involves particle nucleation, growth, coagulation, agglomeration and also oxidation, since the burnup of soot particles once they are formed is a significant process.

Much more research is needed along such lines, the focus being on processes occurring during fuel consumption in fuel-rich flames, an area in need of much further clarification.

Understanding of the problem of production of oxides of nitrogen is in much better shape as a consequence of its greater simplicity and extensive research - the problem is by no means simple, but it is less complicated than the fuel chemistry problem. It becomes necessary to add nitrogen chemistry to the flame chemistry, and this can greatly increase the number of elementary steps. There are various tabulations of rates of the important elementary steps (Miller, Bowman, 1989). One scheme adds 52 elementary steps to include the necessary

nitrogen chemistry (Hewson, Bollig, 1996; Hewson, Williams, 1999). The chemistry in this case can become fairly complicated.

A simplification associated with pollutant production is that the pollutants typically are present in trace concentrations and do not modify the main flame structure. The flame structure can be determined in advance, ignoring the pollutants, and the pollutants can be addressed afterwards. Since pollutant production arises from specific species in the flame, however, reasonable prediction can require relatively detailed knowledge of flame structure. Reduced chemistry can help in sorting out ideas here, as well.

For example, for NO production, the simplest reduced-chemistry step is $2\text{N} + \text{O}_2 \rightleftharpoons 2\text{NO}$ proceeding at the sum of the rates of the elementary steps $\text{O} + \text{N}_2 \rightleftharpoons \text{NO} + \text{N}$, which is followed by $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$ in the thermal mechanism, $\text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N}$; also followed rapidly by $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$; as well as later conversion of HCN to NO, the prompt mechanism) and steps that follow $\text{O} + \text{N}_2 + \text{M} \rightarrow \text{N}_2\text{O} + \text{M}$.

The CH comes from the fuel chemistry, primarily from acetylene through methylene, and to obtain reasonable CH concentrations it has been found desirable to take acetylene out of steady state, adding to the fuel chemistry the overall step $2\text{CO} + \text{H}_2 \rightleftharpoons \text{C}_2\text{H}_2 + \text{O}_2$ the rate of which is largely that of $2\text{CH}_3 + \text{M} \rightarrow \text{C}_2\text{H}_6 + \text{M}$.

Peak flame temperature must in general be below about 1800 K for the prompt contribution to begin to be dominant; the thermal contribution is more strongly temperature dependent. The prompt mechanism becomes of concern in designs attempting to reduce NO emissions to very low levels.

6. SELF-ACCELERATION OF FLAMES – FLAME INSTABILITIES – VELOCITY OF PROPAGATING FLAMES

Flames instabilities

It is well known that a flame propagating in a tube rather seldom shows as a planar front, but acquires a curved or even corrugated shape, which is accompanied by considerable increase of the flame velocity. Similarly, a spherical flame spreading out from the ignition point appears not as the outward propagating smooth spherical front but as a multiple-scale resembling a fractal structure. It was well established that the flame is intrinsically unstable against small perturbations bending the flame front. There are two principle mechanisms of the flame instability. The first one is known as the hydrodynamic instability discovered by Darrieus and Landau (LD instability). The LD instability is inherent to all flames in gaseous mixtures since the instability is related to the gas expansion in exothermal reactions. The expansion coefficient is the ratio of the fuel density and the density of the burnt matter and for laboratory flames $\Theta = \rho_f / \rho_b \approx 6 \div 10$.

Since thickness of a flame front is much smaller than any hydrodynamic length-scales, in the first approximation the flame front can be treated as a surface of zero thickness separating the fresh fuel and the burnt matter and propagating with a constant velocity U_f with respect to the fuel. In this approximation Darrieus and Landau (Landau, 1944; Darrieus, 1945) found that the flame front is unstable against small perturbations bending the front with the growth rate of perturbations

$$\sigma = \Gamma U_f k, \tag{19}$$

where, $k = 2\pi / \lambda$ is the perturbation wavenumber (λ is the wavelength), and numerical

factor depends on the expansion coefficient $\Gamma(\Theta) = \frac{\Theta}{\Theta + 1} \left(\sqrt{\Theta + 1} - 1/\Theta - 1 \right)$.

If dissipations (viscosity, thermal conductivity) are taken into account, then the growth rate is limited for a short wavelength (Clavin and Williams, 1982; Pelce and Clavin, 1982; Liberman et al., 1993, 1994). In the linear theory, the growth rate of small perturbations becomes

$$\sigma = \Gamma U_f k \left(1 - \frac{k \lambda_c}{2\pi} \right), \quad (20)$$

where λ_c is the cut-off wavelength for which the instability is suppressed by thermal conduction. For the case of unit Lewis number and the constant thermal conduction coefficient the cut-off wavelength is given by the formula

$$\lambda_c = \frac{\pi L_f (\Theta - 1)}{\Gamma \sqrt{\Theta + 1 - 1/\Theta}} \left(1 + \Theta \ln \Theta \frac{\Theta + 1 + 2\Gamma}{(\Theta - 1)^2} \right). \quad (21)$$

The cut-off wavelength depends only slightly on thermal expansion, and for the flames with $\Theta = 5 - 10$, it takes value $\lambda_c \approx 20L_f$. The fastest growing perturbations have wavelength $\lambda = 2\lambda_c \approx 40L_f$.

In the presence of a gravitational field the LD instability is amplified by the Rayleigh-Taylor (RT) instability for the flames propagating upwards ($g > 0$), and the gravity plays stabilizing role downwards propagating flame ($g < 0$). Taking this into account, new promising possibilities to govern the burning rate open for flames interacting with acoustic waves.

Velocity of a curved propagating flame

It was pointed out above that one of the main reasons for a flame to lose its initially planar (smooth) configuration is the flame instability. Because of the instability, small perturbations of a flame front grow and bend the front. Saturation of the perturbations growth is due to nonlinear effects, which leads to formation of stationary curved flames and to a considerable increase of the flame velocity compared to the velocity of a planar flame. Outcome of the LD instability at the nonlinear stage may be wrinkling of the initially planar flame front, which may lead to the stationary cellular structure of the freely propagating flames (Fig.2), or to a smooth curved shape of the flame propagating in tubes (Fig.3). Since the surface area of a wrinkled flame increases with the wrinkling development, the flame consumes more fuel per unit time and propagates faster. Typically, in the case of $Le < 1$ (usually – lean flames) the scale of cellular structure induced by the diffusive instability is controlled by the maximum growth rate of small perturbations. The LD instability favors large-scale structure controlled by the hydrodynamic length-scales of the system, for example, tube diameter.

The shape and velocity of a laminar flame traveling through a combustible gas in many respects depends upon hydrodynamic instability arising at a planar flame front. A planar flame front becomes spontaneously curved due to the LD instability and may, in principle, acquire a steady cellular structure. Curved shapes of flames in tubes have been observed both in experimental studies and in numerical simulations (Liberman.et.al.1994, Kadowaki, 1995, Kadowaki, 1995a Denet, Haldenwang, 1995, Bychkov.et.al., 1996, Bychkov.et.al., 1997, Bychkov.et.al., 1997a, Kadowaki, 1999, Travnikov.et.al, 1999). Typical evolution of the initially planar flame propagating in a tube is illustrated in Fig.3.

While the wrinkling of flame front is well documented experimentally, there have been many controversies in both physical origin and modeling of this phenomenon (Bychkov and Liberman, 2000). Difficulties encountered in trying to obtain a closed description of flame propagation are first of all conditioned by the fact that the process is essentially nonlinear and nonlocal. The gas flows both upstream and downstream are strongly affected by the flame

front structure itself. One of the most important features of non-locality of the flame propagation is the vorticity produced by the curved flame downstream, which highly complicate the downstream flow structure (Fig.4). The main reason underlying the complexity of the problem is the hydrodynamic instability of flames. In view of this, evolution of the flame front cannot be prescribed in advance and should be determined in the course of joint analysis of the flow dynamics outside the flame front and the heat diffusion inside. Nonlinear interaction of different perturbation modes under the smoothing influence of thermal conduction leads to the formation of a steady curved flame front with the curvature radius of the order $20L_f$. This estimate follows from the linear theory of the LD-instability, where it corresponds to the cut-off wavelength λ_c . Notice, that analysis of the nonlinear development of the LD-instability, in particular, formation of the stationary flame configurations, is highly complicated since it cannot be carried out perturbatively for arbitrary gas expansion. From the mathematical point of view, perturbation analysis is inapplicable because the assumptions of weak nonlinearity and stationarity of the flame contradict each other. Using them simultaneously turns out to be inconsistent except for the case, $\Theta \Rightarrow 1$. Only in the case of small gas expansion can the problem be treated both perturbatively and locally, since then the amplitudes of perturbations remain small compared to their wavelengths at all stages of development of the LD-instability and the flow is potential both upstream and downstream in the lowest order in $(\Theta - 1) \rightarrow 0$. In this a weakly nonlinear approximation Sivashinsky (Sivashinsky, 1977) has derived the integro-differential equation known as the Michelson-Sivashinsky equation, which describes the evolution of the shape of a flame front. In general case, while the flow is potential upstream where the flow equations can be easily solved, the general solution of the flow equations downstream for the burnt matter cannot be written in a closed form, because the value of the vorticity generated by a curved flame downstream is not known in advance. The presence of vorticity makes the problem essentially nonlocal, since, the value of the pressure field at the flame front is a functional of the velocity field in the bulk.

For the expansion coefficients $\Theta = 6 \div 10$, corresponding to real flames, the nonlinear equations describing curved stationary (Kazakov and Liberman, 2002(a,b)) and nonstationary (Kazakov and Liberman, 2002(c)) flames were obtained recently in a closed analytical form. The velocity amplification of a curved flame is

$$U_w = U_f \left[1 + \frac{(\theta - 1)^2}{4\theta(\theta + 1)} \right], \quad (22)$$

for 2D flames, and about 2 times greater for the 3D flames compared to the flames propagating in 2D channel.

It should be emphasized that the direct numerical simulation of flame propagation for a system of practical interest is a very difficult task even using the most powerful modern computers. For correct calculation of the flame velocity, one has to resolve chemical zone within the flame front, which is about 0.01 mm for typical hydrocarbon flames, while the characteristic length scale of the hydrodynamic flow varies from 10 cm for engines, to several meters for gas-turbine combustors. The problem is even more difficult in the case of turbulent combustion where all the important scales of the turbulent flow need to be resolved. This is why researchers are forced to use a simplified models combined with analytical methods.

Fractal structure of expanding spherical flames

Outcome of the LD instability at the nonlinear stage may be wrinkling of the initially planar flame front, which may lead to the stationary cellular structure of the freely propagating flames, or to a curved shape of the flame propagating in tube. If the cell size is large

compared to the cut-off wavelength, then the cellular flame in turn may become unstable against the LD instability on a smaller scale. As a result of this secondary LD instability a fine structure arises on the larger cells. If the largest instability length scale exceeds the cut-off wavelength by many orders of magnitude, then as a result of such cascades of the secondary instabilities consisting of small cells imposed on larger cells, a fractal structure may develop at the flame front (Gostintsev.et.al. 1988, Filiand, Sivashinsky, 1994, Blinnikov. Sasorov, 1996, Bychkov, Liberman, 1996, Bychkov and Liberman, 2000). This picture is consistent with the fascinating experimental studies by Gostintsev.et.al.1988, which indicated that the initially smooth freely expanding spherical flames undergoing wrinkling due to well-developed hydrodynamic instability on the large scales, expand with a noticeable acceleration. It was found that growth of the average radius with the 3/2 power of time is universal for all the spherically expanding flames

$$\bar{R} \approx At^{3/2} \quad (23)$$

The fractal structure of a flame front may be described as cascading humps and cusps: humps and cusps of smaller scales develop on humps of large scales and so on. The general idea of the process may be understood from the Koch curved constructed as a cascade of triangles (Mandelbrot, 1983).

Taking into account similarity of a fractal flame and the Koch curve one can consider a curved stationary flame as one step of the cascade similar to the Koch triangles. In that case one should interpret the curved stationary flame as the generator of a fractal flame structure (Bychkov and Liberman, 1996). In a simple model of an infinitely thin flame front the increase of the flame velocity is equal to the increase of the flame front surface. If a fractal flame has an excess d (a fractal dimension $2 + d$), then the resulting velocity of flame U_w depends on the hydrodynamic length scale, which is the flame radius in the case of spherical flame, $U_w = dR/dt \propto R^d$. This dependence corresponds to self-similar acceleration of a fractal flame

$$R = C_f t^\alpha, \quad (24)$$

with the self-similarity exponent $\alpha = 1/(1-d)$ which is related to the fractal excess, d . The self-similarity exponent, $\alpha = 3/2$, implies the fractal excess $d = 1/3$ and the fractal dimension of the flame 2.33. The corresponding fractal dimension calculated from the flame velocity increase on one step of the cascade of the secondary LD instability, using Eq.(22) gives values 1.2 and 2.3 for 2D and 3D flames respectively, which is consistent with the experiments.

For the flames characterized by moderate turbulence level and high Damköhler number, reaction in premixed flames occurs in a thin sheet known as flamelet. Mandelbrot (1983) suggested that surfaces of constant properties of passive scalars in homogeneous and isotropic turbulent flows possess fractal character. These surfaces should exhibit fractal behavior within a range of scales, which is limited at the low end by the Kolmogorov scale and should be bounded by the large scales of the flow at the high end. The latter can be by order of magnitude, the integral length scale of turbulence, or radius of a spherical flame, for example. It is interesting that in this case the same fractal dimension arises in turbulent flames as for expanding spherical flames. Idea that the LD hydrodynamic instability may act as a generator of the Kolmogorov turbulence seems plausible especially as 3/2 power law is consistent with the scaling law followed from Kolmogorov theory. In contrast to spherical flames, the morphology of the flames propagating in tubes is essentially different, since cascade corrugations merge forming a single cusp whose size is controlled by the tube radius.

There is no final solution to the problem of fractal dimension of a flame front so far; it is still unclear if the fractal flame dimension is a universal parameter. A number of works have

been published (Filiand et al., 1994; Rahibe et al., 1995; Bravo and Garcia-Senz, 1995; Blinnikov and Sasorov, 1996; Kupervasser et al., 1996; Galanti et al., 1998 in attempt to understand fractal nature of laminar and turbulent flames. Results of the recent direct numerical simulation (Liberman, Valiev, et al, 2003) shown in Fig. 6, 7 are seemed to confirm the fractal idea. As is seen from Fig.6, the shape of spherically expanding flame shows amazing similarity of a fractal flame and the Koch triangles. Also, after formation of a fractal structure the regime of the flame propagation approaches the self-similar acceleration regime Eq.(23).

7. DETONATION

Contrary to the deflagration (slow combustion-flame) discussed above, where the propagation through the combustible gas is due to the heat transfer by thermal diffusion, detonation is entirely different regime of propagation of combustion, involving shock waves. The shock wave traveling through the combustible mixture compresses and heats the gas behind the shock front. If the shock wave is sufficiently strong, then the rise in temperature may be sufficient to ignite combustion behind the shock front. Thus, detonation waves are shock waves which are sustained by the energy of the chemical reaction that is initiated by the shock compression and heating. For example, the temperature rise behind the shock wave propagating with velocity $D=2800m/sec$ through $2H_2+O_2$ gas mixture at room temperature is

$$\Delta T = \frac{D^2}{2C_p} \left\{ 1 - \frac{(\gamma-1)^2}{(\gamma+1)^2} \right\} \cong 1800K, \quad (25)$$

which is enough to ignite reaction.

There is no space here to go into details of the detonation theory. The modern detonation models used is the *Zel'dovich-von Neumann-Döring* model (ZND-model). According to the ZND model a detonation consists of a shock wave traveling at the Chapman-Jouguet (CJ) velocity followed by a reaction zone. The conditions behind the leading shock wave are different from the CJ final conditions, in particular, the pressure and density are much higher than that for CJ. The shock compresses and heats the combustible mixture, which is ignited and begins to react. The overall fuel oxidation consists of a relatively long induction period during which the temperature and pressure of the combustible mixture remains almost constant, followed by a rapid release of chemical energy and temperature increase. The shock wave which is characterized by a very thin front (of order of the molecule mean free path) is followed by the reaction zone – layer moving with the shock, in which combustion is occurring. It is clear that the width of this layer, which is about the speed of the shock wave multiplied on reaction time, τ_b is much larger than the width of a flame in the same mixture, $L_f \cong \tau_b U_f$. Thus, the thickness of the detonation wave is about D/U_f times greater than the flame thickness. For example, while the width of the flame in hydrocarbon propagating with velocity $U_f \approx 40cm/s$ is $L_f \approx 10^{-2}cm$, the corresponding thickness of detonation wave is approximately 1 meter. This simple estimate explains that the rise of the temperature in a small spot will ignite a flame but not a detonation.

Gaseous detonation waves have been studied experimentally for many years. Detonation limits, propagation rates, and initiation properties have been examined for many fuel-oxidation mixtures. Theoretical description of detonation shows how hydrodynamic and chemical kinetic processes interact in the detonation waves. The weakest point in the theoretical description and in the existing detonation models is the same as for the flames: this is sub-models for chemical kinetics. Since the induction time plays a crucial role for all models, the lack of reliable chemical kinetic models has been a serious problem.

The first applications of detailed models to compute the detonation induction time using detailed hydrogen-oxygen mechanism have been made in relatively recent time. This became possible due to the simplicity of the hydrogen-oxygen mechanism and the availability of reliable data for the majority reactions involved (see Section 4). For a more complex gas mixtures, for example, hydrocarbon fuels, quantitative analysis is limited by the lack of reliable chemical kinetic models; rates and constants for many reactions are known with a poor accuracy. Difficulties in handling the problem are similar to that the researchers have for the flame modeling when reliable models require coupling 3D hydrodynamic with detailed chemical kinetics.

Deflagration-to-Detonation transition

Mechanism of the transition from deflagration to detonation remains one of the most challenging in combustion science. Although significant progress has been achieved in the past years, a comprehensive first-principle understanding of the phenomena is still lacking. It has long been observed that deflagration-to-detonation transition is reluctant to occur in open and obstacle-free systems, but presence of the walls, confined combustion in closed vessels are favorable for the transition.

In a rigorous sense a stationary flame front does not exist without losses, since the fuel always reacts ahead of the flame front though with a very low rate (Zeldovich, 1980; Zeldovich et al., 1985). In reality one may usually neglect the spontaneous reaction in an unbounded fuel due to the large activation energy compared to the initial fuel temperature. Formally this is equivalent to the implicit assumption about some small heat losses in the fresh fuel. The situation is different for flames under confinement. The pre-compression of the fuel ahead of the flame front raises the fuel temperature and density, which may result in a strong decrease of the reaction time ahead of the flame front. Spontaneous development of the reaction ahead of the flame front traveling in a closed tube may trigger detonation at the opposite tube end. For a gaseous combustible in a tube, a flame can experience a transition to detonation only through an unsteady or nonplanar process. Both, expansion of the burned gases and instabilities accelerate the flame and cause two processes that initiate transition to a detonation: emitting pressure waves that propagate in the direction of flame and turbulization. The pressure waves emitted by an asymmetrical curved flame converge to the corner of the tube close to the wall, which the cusp of the curved flame front touches. The pressure waves compress the fresh mixture and rise its temperature. Kinetic energy of the shock is cumulated at the point of convergence. The fuel temperature is maximal at the cumulating points and it is these points, where the detonation starts. The temperature increase can be great enough at the point of convergence to generate local explosions that develop into new propagating deflagration waves moving outward from cumulating points. Eventually, pressures in excess of final detonation pressures develop, and detonation then propagates through the rest of the combustible mixture in the tube.

A criteria of the detonation triggering ahead of the flame front can be expressed as a condition of a self-accelerating reaction ahead of the flame front: the heat release in the reaction must be larger than the adiabatic cooling in the emitted sound wave:

$$\left. \frac{dT}{dt} \right|_{chem} > \left. \frac{dT}{dt} \right|_{sound}. \quad (26)$$

On the basis of Eq. (26) one can calculate position of the flame front when the detonation is triggered as a function of the tube length (Lieberman et al., 1998).

White dwarf burning in Supernova events

An interesting example of flame dynamics in a strong gravitational field is propagation of thermonuclear flames from the centre of an exploding white dwarf in thermonuclear Supernovae, which are also known as Supernovae of type I. It is a general belief that the thermonuclear Supernovae emerges as a result of explosion of carbon-oxygen white dwarfs accreting mass. Such a white dwarf has burnt already hydrogen and helium, so that the gravitational pressure inside the star is balanced by the pressure of degenerate electrons, which is almost independent of the star temperature. If the white dwarf accretes mass, then the temperature at the white dwarf centre increases and the carbon reaction may be ignited, which happens, when the central temperature of the white dwarf grew above $6.6 \cdot 10^8$ K. At the moment of the thermal run-away the typical central density of the white dwarf is about $\rho_c = 3 \cdot 10^9$ g/cm³ and the star mass is close to the Chandrasekhar limit $M_{WD} = 2.8 \cdot 10^{33}$ g. Subsequently thermonuclear burning can propagate either in deflagration regime (flame) or in detonation (supersonic) regime. The choice of the burning regime is important in the theory of thermonuclear Supernovae, because it affects the chemical composition of the “ashes” and the total energy of the explosion.

Since the characteristic scale of the problem is of order of 10^3 km, which is much larger than the thickness of detonation and deflagration fronts, which are of order of $10^{-5} - 10^{-3}$ cm and < 0.1 cm, respectively, direct numerical simulation can not answer the question of hydrodynamic regime of white dwarf burning: the grid is too rough to determine the hydrodynamic regime of burning, and the choice of the burning regime becomes inevitably an artifact of a particular simulation.

The flame may be ignited in white dwarfs by a reacting volume of a size of 0.3 m. On the contrary, the reaction has to start on scales comparable to the size of the hot center (about 1 km) of the white dwarf in order to ignite the detonation (Bychkov and Liberman, 1995). As a result flame always starts first in the Supernova explosions. As the flame propagates it forms a bubble of burnt matter separated from the cold fuel by the flame front, which is the surface of the bubble. The density of the burnt matter inside the bubble is smaller than the density of the surrounding fuel, therefore the bubbles are coming to the surface of the star. The bubbles formed from the burned matter are travelling to the surface faster than they grow when radius of bubbles exceeds $R > 10$ km. The bubble radius is much smaller than the radius of the hot central part of the white dwarf estimated as 100 km. Similar estimates show that the mass of the burnt matter in the bubble of burnt matter is negligible (less than 0.1%) in comparison with the total mass of the hot fuel in the center of the star. Thus the deflagration stage of white dwarf burning is asymmetrical and the hot central part of the white dwarf remains essentially unburned. The unburned fuel at the center of the white dwarf may explode later leading to the detonation regime of burning.

Detonation dynamics in white dwarfs is also strongly affected by hydrodynamic instabilities. Particularly, it has been shown (Kriminski et al., 1998) that thermonuclear detonation is unstable against 1D pulsations of the front for sufficiently large densities of the thermonuclear fuel of the white dwarfs $\rho > 2 \cdot 10^7$ g/cm³. The instability is similar to the instability of a detonation wave in a chemical combustible with large activation energies of the reaction (Zaidel, 1961; Erpenbeck, 1962; Zaidel and Zeldovich, 1963), which leads to self-quenching of the detonation (He and Lee, 1995; Clavin and He, 1996). Thus, the detonation in white dwarfs cannot propagate at high densities $\rho > 2 \cdot 10^7$ g/cm³: instead the detonation regime of burning becomes possible only when the white dwarf density has sufficiently decreased due to pre-expansion on the deflagration stage of the star burning.

8. Explosions

Typically explosion is called a process of a violent exothermal reaction where the temperature and pressure are raised very fast compared to the time scales that humans usually consider as ordinary. The explosion can be triggered by an ignition source, or it may develop spontaneously, for example, if exothermal solids are stored in piles that are too large. The term explosion is derived from damaging overpressures that occur.

A well-know example of explosion is undesirable knocking in engine combustion. This abnormal combustion known as knock, which got this nickname from the noise that is transmitted from the colliding of the multiple flame fronts and the increased cylinder pressure that causes the piston, connecting rod and bearings to resonate, has been the limiting factor in internal combustion engine power generation since the discovery of the Otto cycle itself. At present it is generally accepted that SI-engine knock is caused by autoignition in the unburned part of the combustion mixture, the end-gas ahead of the propagating flame, which has not been reached by the flame. Autoignition of the end-gas occurs when the temperature and pressure exceed a critical limit so that comparatively slow reactions, realizing moderate amounts of heat, transform into ignition and fast energy release. Due to the locally rapid energy release, pressure gradients are developed in the combustion chamber, causing pressure oscillations, which results in knocking sounds. It is thus a direct constraint on engine performance. It also constrains engine efficiency, since by effectively limiting the temperature and pressure of the end-gas, it limits the engine compression ratio.

Typically explosion is called ignition of the combustion which is accompanied by a loud noise or clap. Why ignition of a natural gas in the kitchen oven does not produce a noise, but ignition of similar amount of the hydrogen-oxygen mixture looks as an explosion? What do they have in common, what are the differences between ignition of a natural gas and hydrogen?

After the moment of ignition, the burning is a flame front spreading out from the ignition point. The flame front represents a piston, which is moving with acceleration, for example, according to Eq. (23) in case of a spherically expanding flame, into the gas at rest. It is known that if a piston is moved into the gas, then a simple compression wave originates at the piston. In course of time the velocity profile in the compression wave steepens (Fig.9), and initial discontinuity – shock wave is formed at some location ahead of the propagating flame (Fig.10). The time and location where the shock wave will be formed are defined by the envelope of the characteristics intersection which are emitted by the piston, and they can be calculated analytically. Let R_{shock} is the co-ordinate of the shock formation, R_{flame} - co-ordinate of the flame front (piston), $D = R_{shock} - R_{flame}$. Ratio of the latter values for the methane and hydrogen flames is

$$\frac{(R_{shock} - R_{flame})_{CH_4}}{(R_{shock} - R_{flame})_{H_2O_2}} \propto \frac{U_f^3(H_2O_2)}{U_f^3(CH_4)} \cong 200 \div 400. \quad (27)$$

In the case of hydrogen ignition, shock wave is formed at about 1 mm ahead of the flame, while flame in methane must travel about 10 cm before the shock will be formed. These simple estimates explain why ignition of a small amount of H_2O_2 is accompanied by a clap and looks like an explosion. Many people know from their kitchen experience know that the gas ignition at the gas-stove-oven can be accompanied by a clap if gas was ignited after it filled considerable part of oven. The above consideration gives explanation of this phenomena.

CONCLUSIONS

There are many different aspects to the subject. Many important issues of combustion are not addressed in the present lecture, such as ignition, flammability, quenching, chain branching, extinction, thermal runaway, stability of detonation, etc., because of limiting space. The number references that have been cited also does not correspond to a thorough review, but the opposite is in fact true. Only a very small amount of the relevant work has been cited, and the choice of the cited papers was motivated either by the limited space or was not motivated. Many of the particular needs for future research directions have been indicated in the previous sections where the specific topics are discussed. It seems desirable, however, to try to give a more general overview of promising directions for future research. To begin with, there is a strong need in improved numerical models that are 3D hydrodynamical models coupled with detailed chemistry. The unknowns lie almost entirely with the fuel chemistry and complexity in coupling detailed chemistry with 3D flow. This is especially true for various hydrocarbon and alternative fuels that have not been studied thoroughly. A great deal of similar work is needed for better understanding deflagration-to-detonation transition. Another problem of considerable interest and industrial application is the flame – acoustic wave interaction. Development of this kind of information will lead, through improved knowledge, to good methods for governing the combustion process, enhance burning thermodynamic efficiency and to decrease pollutant emission. This work must be both experimental, theoretical and computational. To develop a thorough and correct description of hydrocarbon combustion is a very challenging and important task.

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FIGURE CAPTIONS

- Fig. 1 (a) Premixed flame structure on the basis of one-step activation energy asymptotic.
- Fig. 1 (b) Structure of a diffusion flame on the basis of one-step activation energy asymptotic.
- Fig. 2 Consecutive Schlieren photographs illustrating formation cellular flame structure.
- Fig. 3 Numerical simulation of a flame shape evolution in a wide tube.
- Fig. 4 Numerical simulation: flow field and vorticity generated by the flame propagating in tube.
- Fig. 5 Numerical simulation: flow field and vorticity generated by the flame propagating in engine cylinder.
- Fig. 6 Consecutive steps of the Koch curve.
- Fig. 7 Numerical simulation showing consecutive configuration of the expanding wrinkled flame.
- Fig. 8 Numerical simulation showing average radius of the expanding spherical flame versus time.
- Fig. 9 Steepening of the compressive part and fluttering of the expansive part in the velocity profile of a simple pressure wave entering gas at rest.
- Fig. 10 Envelope of the straight characteristics of the compression wave produced by a uniformly accelerated piston.

MOVIE

Numerical simulation of the flame propagating in tube.
Numerical simulation of combustion in an engine cylinder.
Numerical simulation of spherically expanding flame.

REFERENCES

- Barenblatt G.I., Zeldovich Ya.B., and Istratov A.G. (1962) Prikl. Mech. Tekn. Fiz. 2, 21.
- Blinnikov S.I. and Sasorov P.V. (1996) Phys. Rev. E 53, 4827.
- Bravo E. and Garcia-Senz D. (1995) Astroph. J. 450, L17.
- Bychkov V.V. and Liberman M.A. (1994) Phys. Rev. Lett. 73, 1998.
- Bychkov V.V. and Liberman M.A. (1995) Astron. Astroph. 302, 727.
- Bychkov V.V. and Liberman M.A. (1995) Astroph. J. 451, 711.
- Bychkov V.V. and Liberman M.A. (1995) Astron. Astroph. 304, 440.
- Bychkov V.V. and Liberman M.A. (1996) Phys. Rev. Lett. 76, 2814.
- Bychkov V.V., Golberg S.M., Liberman M.A. and L.E. Eriksson (1996) Phys. Rev. E 54, 3713.
- Bychkov V.V. and Liberman M.A. (1997) Phys. Rev. Lett. 78, 1371.
- Bychkov V.V. and Liberman M.A. (1997a) J. Exp. Theor. Phys. 84, 281.
- Bychkov V.V., Kleev A.I., Liberman M.A., and Golberg S.M. (1997) Phys. Rev. E 56, R36.
- Bychkov V.V., Golberg S.M., Liberman M.A. and Kleev A.I., (1997a) Comb. Sci. Tech. 129, 217.
- Bychkov V.V., Kleev A.I., and Liberman M.A. (1998) Comb. Flame 113, 470.
- Bychkov V.V. and Liberman M.A. (2000) Physics Reports, 325, No.4-5.
- Clavin P. and Williams F.A. (1982) J. Fluid Mech. 116, 251.
- Darrieus, G. (1945) Propagation d'un front de flamme, presented at Le congrès de mécanique appliquée, unpublished.
- Denet B. and Haldenwang P. (1995) Comb. Sci. Tech. 104, 143.
- Erpenbeck J.J. (1962) Phys. Fluids 5, 604.
- Filiand L., Sivashinsky G.I. and Frankel M.L. (1994) Physica D72, 110.
- Frankel M.L. and Sivashinsky G.I. (1982) Comb.Sci.Tech. 29, 207.
- Galanti B., Kupervasser O., Olami Z., and Procaccia I. (1998) Phys. Rev. Lett. 80, 2477.
- Gostintsev Y.A., Istratov A.G. and Shulenin Y.V. (1988) Comb. Expl. Shock Waves 24, 70.
- He L. and Lee J.H.S. (1995) Phys. Fluids 7, 1151.
- Hewson J. C., Bollig M. (1996) Reduced mechanisms for NO_x emissions from hydrocarbon diffusion flames. Twenty-sixth Symposium (International) on Combustion. The Combustion Institute, Pittsburgh, p. 2171.
- Hewson J. C., Williams F. A. (1999) Combust Flame, 117, 441.
- Kazakov K. A. and Liberman, M. A. (2002-a) Phys. Rev. Letters 88, 064502-1.
- Kazakov K. A. and Liberman, M. A. (2002-b) (Phys. Fluids 14, 1166.
- Kazakov K. A. and Liberman, M. A. (2002-c) Comb. Sci. Tech. 174, 157.
- Kriminski S.A., Bychkov V.V. and Liberman M.A. (1998) New Astron. 3, 363.

Kupervasser O., Olami Z., and Procaccia I. (1996) *Phys. Rev. Lett.* 76, 146.

Landau L.D., *Acta Physicochimica (URSS)* 19, 77 (1944).

Landau L.D. and Lifshitz E.M. (1987) *Fluid Mechanics*, Pergamon Press, Oxford

Lieberman M.A., Bychkov V.V., Golberg S.M. (1993) *J. Exp. Theor. Phys.* 77, 227.

Lieberman M.A., Bychkov V.V., Golberg S.M. and Book D.L. (1994) *Phys.Rev. E* 49, 445.

Lieberman M.A., Golberg S.M., Bychkov V.V., and Eriksson L.E., (1998) *Comb. Sci. Tech.*, 136, 221.

Lieberman M.A., Valiev D., *Phys. Rev. E* (2003) in press.

Mandelbrot B.B. (1983) *The Fractal Geometry of Nature*, Freeman, San Francisco

Manheimer W.H., Colombant D.G., and Gardner G.H. (1982) *Phys. Fluids* 25, 1644

Manheimer W.M. and Colombant D.R. (1984) *Phys. Fluids* 27, 983

Pelce P. and Clavin P. (1982) *J. Fluid Mech.* 124, 219.

Rahibe Z., Aubry N., Sivashinsky G. and Lima R. (1995) *Phys. Rev. E* 52, 3675.

Shelkin K.I. (1940) *Zh. Eksp. Teor. Fiz.* 10, 823.

Sivashinsky G.I. (1977) *Acta Astronaut.* 4, 1177.

Timmes F.X. and Woosley S.E. (1992) *Astroph. J.* 396, 649.

Travnikov O.Yu., Lieberman M.A., and Bychkov V.V. (1997) *Phys. Fluids* 9, 3935.

Zaidel R.M. (1961) *Doklady AN SSSR* 136, 1142.

Zaidel R.M. and Zeldovich Ya.B. (1963) *Prikl. Mech. Tekh. Fiz.* 6, 59.

Zeldovich Ya.B. and Frank-Kamenetski D. A. (1938) *Acta Physicochimica URSS* 9, 341.

Zeldovich Ya.B. and Rozlovski A.I. (1947) *Doklady Acad. Nauk SSSR* 57, 365.

Zeldovich Ya.B.(1966) *Prikl. Mekh. Tekh. Fiz. N.1*, 102.

Zel'dovich YB, Frank-Kamenetskii DA. *Zhur Fiz Khim* (1938) 12, 110.

Zel'dovich YB, Semenov NN. *Zhur Eksp Teor Fiz* (1940) 10, 1427.

Zeldovich Ya.B. (1980) *Comb. Flame* 39, 211

Zeldovich Ya.B., Istratov A.G., Kidin N.I. and Librovich V.B. (1980) *Comb. Sci. Tech.* 24, 1

Zeldovich Ya.B., Barenblatt G.I., Librovich V.B., Makhviladze G.M. (1985) *The Mathematical Theory of Combustion and Explosion*, Consultants Bureau, NY.

Williams F. A. (1985) *Combustion Theory*, 2nd ed., Benjamin/Cummings, Menlo Park, California.