Classification of dynamic problems of the theory of combustion and explosion

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Introduction

The current state of the theory and practice of combustion and explosion of gases and fuel-air mixtures in limited volumes and internal combustion engines is characterized by the increasing complexity of the scientific and technical problems being solved and the dynamical problems under consideration. In considering a particular problem, it is important to classify it as a class of dynamic problems in the theory of combustion. This is necessary for the analysis and use of previous scientific experience in solving similar dynamic problems from the point of view of combustion theory. Unfortunately, such a classification of dynamic problems in the theory of combustion according to our data is currently absent [1].

Another important problem is the need for an adequate description of the most complex hydrodynamic, thermodynamic, chemical and physical processes (including the processes of energy, momentum and mass transfer) that occur during explosions of gases in limited volumes and in the combustion of fuel and air mixtures in internal combustion engines of various types. It is important not only qualitative, but also quantitative description of the processes under consideration.

Classification of dynamic problems

In dynamic problems of the theory of combustion, there are (or should be) similarity criteria, which are the ratio of the characteristic times of the process. The question arises, were anyone considering similar problems before? This will be the subject of our analysis. We note that usually in dynamic problems of combustion theory there are changed pressure, temperature and volume. We restrict the circle of our consideration to the following physical processes and, correspondingly, the characteristic times that usually occur in dynamic problems.

1) The characteristic time of an isothermal volumetric chemical reaction (the time over which at the initial reaction rate

$$W(0)=\left(A^*\right)^s k_0 \exp\left(-\frac{E}{RT^*}\right)$$

with a thermal effect per unit volume $QA^*=c_p\rho\left(T_{\max}-T^*\right)$ the temperature in the volume under consideration is increased by one characteristic interval $\Theta=R\left(T^*\right)^2/E$) [1, 6]

$$t_V = \frac{A^*}{W(0)} = \left(A^*\right)^{1-s} k_0^{-1} \exp\left(\frac{E}{RT^*}\right), \quad (1)$$

where $A*$ - the concentration of the reacting component of the mixture, s - the order of the chemical reaction, k_0 - the pre-exponential of the rate constant, E - the activation energy, R - the universal gas.

2) The characteristic time of frontal combustion (including turbulent combustion with a flame turbulence factor χ)

$$t_f = \frac{L}{\chi S_u^*}; \quad (2)$$

3) The characteristic time of heat transport or heat transfer (the ratio of the chemical energy of the system QA^*V, or per unit heat exchange area F $QA^* V/F = QA^* L$ (*under the condition* $V \approx FL \approx L^3$), to the rate of its loss by thermal conductivity or heat transfer, with a temperature gradient or a temperature difference equal to one characteristic interval $\Theta = R\left(T^*\right)^2 / E$

$$t_\lambda = \frac{QA^*V}{\lambda L \Theta} = \frac{QA^* L^2}{\lambda} \cdot \frac{E}{R\left(T^*\right)^2}, \quad (3)$$

$$t_\alpha = \frac{QA^*V}{\alpha F \Theta} = \frac{QA^* L}{\alpha} \cdot \frac{E}{R\left(T^*\right)^2}. \quad (4)$$

4) The characteristic time for the outflow of gas from the volume under consideration (under the critical discharge regime)

$$t_0 = \frac{V}{gFa^* z}, \quad (5)$$

where gF - effective discharge cross-section, a^* - sound velocity, z - the parameter of the discharge regime.

5) The characteristic time of the compression process (of the motion of the piston in the engine and in the adiabatic compression setup of the "adiabatic gun")

$$t_m = \frac{1}{2\pi n_0}, \quad (6)$$

$$t_p = L\sqrt{\frac{m_p}{2 p_i V_i}}; \quad (7)$$

where n_0 - crankshaft speed, m_p - piston mass, L - gun tube length, p_i, V_i - initial value of pressure and working volume.

6) The characteristic time of temperature change of the enclosing surfaces (the rate of heating or cooling $w = (T_0 - T_i)/t$) per characteristic temperature interval

$$t_w = \frac{\Theta}{w} = \frac{R\left(T^*\right)^2}{wE}\,. \tag{8}$$

The criteria of classic thermal explosion

Among the dynamic problems of *combustion theory* considered earlier, the problems of thermal explosion (TE) are the most known. In the nonstationary (developed by NN Semenov [2-7]) and in the stationary (developed by DA Frank-Kamenetskii [7-11]) theories of thermal explosion, the corresponding similarity criteria κ and δ appear. They bear the names of the authors

$$\kappa = \frac{t_\alpha}{t_V} = \frac{E}{R\left(T^*\right)^2} \cdot \frac{QV}{\alpha F} k_0 \left(A^*\right)^s \exp\left(-\frac{E}{RT^*}\right), \tag{9}$$

$$\delta = \frac{t_\lambda}{t_V} = \frac{E}{R\left(T^*\right)^2} \cdot \frac{QL^2}{\lambda} k_0 \left(A^*\right)^s \exp\left(-\frac{E}{RT^*}\right). \tag{10}$$

These similarity criteria, as seen from (1), (3) and (4), are the ratio of the characteristic times of the process, namely, the heat transport or heat transfer time to the characteristic time of a volumetric chemical reaction (volumetric combustion). Criteria (9) and (10) are essentially equivalent and differ in the laws of heat transfer.

Criterion of dynamic TE

The theory of thermal explosion during heating or cooling is developed in [12-15], the main parameter (the similarity criterion) in which is the ratio of the characteristic time of the bulk chemical reaction to the scale of the temperature change (expressed in units of the characteristic interval)

$$\omega = \frac{t_V}{t_w} = \frac{wE}{R\left(T^*\right)^2} \cdot \frac{\left(A^*\right)^{1-s}}{k_0} \exp\left(\frac{E}{RT^*}\right). \tag{11}$$

In [16, 17], the problems are considered in which a thermal explosion develops as a result of the presence of chemical and mechanical heat sources in the system. If we introduce a parameter characterizing the heating rate from a mechanical source and the corresponding heating time by one characteristic interval of the form (8), we obtain a similarity criterion that completely coincides with the criterion (11).

Criterion for flame propagation limits

It is known the problem, that was considered Ya.B. Zeldovich [1, 18, 19], of the flame propagation limit in channels, which includes the similarity criterion

$$\mathrm{Pe}_f = \frac{t_\lambda}{t_f} = \frac{QLA^* S_u^*}{\lambda} \cdot \frac{E}{R\left(T^*\right)^2}, \tag{12}$$

which is the ratio of the characteristic times of heat transfer and frontal combustion.

Criteria for combustion in vented vessels

In the problems of gas combustion in depressurized vessels, for example, problems on the protection of vessels [20 22], there is a criterion that is the ratio of the characteristic times of frontal combustion and discharge

$$\mathrm{B}_0=\frac{t_f}{t_0}=\frac{L}{\chi S_u^*}\cdot\frac{gFa^*z}{V}, \tag{13}$$

which in the problem of gas combustion in the system of two communicating vessels considered by us is presented in the form [23, 24]

$$\mathrm{B}_\Omega=\frac{\mathrm{B}_0}{0.62J_e}=\frac{gFa^*}{V^{2/3}\chi S_u^*}\cdot\frac{z}{J_e}. \tag{14}$$

Criteria for the competition between frontal and volumetric combustion

In [25, 26] we considered the problem of self-ignition of a gas in front of a flame front in a closed vessel during the propagation of a divergent spherical flame. By an analytical solution, a critical condition is found for the similarity criterion of the process under consideration, namely, a criterion is obtained that is the ratio of the characteristic times of frontal combustion and the bulk chemical reaction

$$u^*=\frac{t_f}{t_V}=\frac{\delta}{\mathrm{Pe}_f}=\frac{L}{\chi S_u^*}\cdot k_0\left(A^*\right)^s\exp\left(-\frac{E}{RT^*}\right). \tag{15}$$

As follows from (15), the similarity criterion is the ratio of the criteria known earlier Frank-Kamenetskii (10) for the stationary theory of thermal explosion and Zel'dovich (13) for the theory of the flame propagation limit in channels. This criterion appears in our works [25, 26] for the first time, that is, the problems of self-ignition in systems with frontal gas combustion have not previously been considered theoretically. Somewhat later, work appeared [27], where a similar process is considered for convergent flames. Then followed the work [28] and others.

In [29] and our subsequent papers [30, 31], self-ignition of a gas due to adiabatic compression in an installation with a free piston (an adiabatic "gun") used to determine the macrokinetics of combustible gas mixtures was considered [32]. The critical condition for self-ignition obtained is proportional to the ratio of the characteristic times of adiabatic compression and the chemical reaction

$$u_p^*=\frac{J_e}{\gamma}\cdot\frac{t_p}{t_V}=\frac{J_e}{\gamma}\cdot L\sqrt{\frac{m_p}{2p_iV_i}}\cdot k_0\left(A^*\right)^{s-1}\exp\left(-\frac{E}{RT^*}\right). \tag{16}$$

It is interesting that the similarity criterion (16) contains as a factor the parameter $J_e/\gamma=E_i-1$ (equal to the expansion coefficient at constant pressure without unity). In terms of physical meaning, the effect of this factor on the process is equivalent to increasing in the characteristic time of the compression process t_p or the characteristic size of the system L, that is, its own heat release as a result of the chemical reaction accelerates the process of self-ignition in the system.

The process of ignition of a mixture in diesel as a problem of a dynamic thermal explosion was considered in [33] and our subsequent studies [34-36]. The critical condition for self-ignition obtained is proportional to the ratio of the characteristic times of the piston motion and the chemical reaction

$$u_m^* = \frac{J_e}{\gamma} \cdot \frac{t_m}{t_V} = \frac{J_e}{\gamma} \cdot \frac{1}{2\pi n_0} \cdot k_0 \left(A^*\right)^{s-1} \exp\left(-\frac{E}{RT^*}\right). \qquad (17)$$

It is easy to see that the criteria (16) and (17) are essentially equivalent and differ only in the law of compression (changes in the volume of the system). We note that until the appearance of our papers [26, 33, 34], criteria of the form (16) or (17) did not appear in the combustion theory. Attempts to consider similar problems by other authors suffer from a one-sided approach; for example, the achievement of a certain critical temperature (self-ignition) is accepted as the autoignition condition, which itself does not follow from theory [37]. Only after the appearance of our paper [26], the authors in [28] corrected their mistake. The authors of [38] were also dealt with similar problems. They investigated the process of adiabatic thermal explosion of gas inclusions in liquids during the collapse of bubbles. In this problem, a criterion of the form (16) or (17) should also appear.

Criteria of autoignition under adiabatic compression

In [39], the dynamics of the process in a ballistic engine, namely, in an installation with a piston freely moving under the action of expanding frontal combustion products, is considered. The determining parameter of the problem (similarity criterion) is proportional to the ratio of the characteristic times of motion of the piston and frontal combustion and can be represented in the form

$$\Delta_p = \frac{J_e}{\gamma} \cdot \frac{t_p}{t_f} = \frac{J_e}{\gamma} \cdot \sqrt{\frac{m_p}{2 p_i V_i}} \cdot \chi S_u^* . \qquad (18)$$

It can be seen that the criterion (18) is a ratio of the criteria (16) and (15) encountered previously. In addition, the paper [39] considers the dynamics of combustion in an engine with ignition from a thermal source (ICE with spark ignition). Here there is a similarity criterion proportional to the ratio of the characteristic times of the compression process in the engine and frontal combustion

$$\Delta_m = \frac{J_e}{\gamma} \cdot \frac{t_m}{t_f} = \frac{J_e}{\gamma} \cdot \frac{\chi S_u^*}{2\pi n_0 L} . \qquad (19)$$

It can be seen that the criterion (19) is the ratio of the above criteria (17) and (15). Note also that the criteria (18) and (19), in essence, are equivalent and differ only in the law of motion of the piston.

Similarity criteria of combined type

Dynamic problems in which more than one similarity criterion is present (three or more characteristic process times) are of particular interest. For example, the problem considered in [40, 41] about self-ignition of a gas ahead of the flame front during combustion in communicating vessels. The main parameter in the problem, which determines the critical conditions for self-ignition in the second vessel, can be represented in the form

$$u_{\Omega}^{*} = \frac{t_f/t_V \cdot \Omega^{1/3}}{1 - t_f/t_0} = \frac{u^{*} \cdot \Omega^{1/3}}{1 - B_0^{*}}. \qquad (20)$$

It can be seen that for a fixed volume ratio, criterion (20) is a function of the criteria (14) and (15).

In our paper [26], a hypothesis was advanced that the considered problem of self-ignition of a mixture ahead of the flame front in a closed vessel is directly related to the problem of "knocking" or detonation in an ICE with spark ignition (which excites researchers for about 100 years and is still finally not solved). That is, the hypothesis is formulated that knocking or detonation in the engine is a problem of competition between the processes of frontal and volumetric combustion. The rigorous formulation of the knock or detonation problem in the engine allowed us to analytically solve the problem of self-ignition and obtain a critical condition of the form [29, 42-48]

$$\Delta_m^{*} = \frac{1}{(t_V/t_f)^{*} + \gamma/J_e \cdot (t_V/t_m)^{*}} = \frac{1}{1/u^{*} + 1/u_m^{*}}. \qquad (21)$$

It can be seen that the criterion (21) is a function of the similarity criteria (15) and (17).

Without pursuing the idea of writing down here all possible criteria for similarity and their combinations, let us dwell on one more interesting problem. The high antiknock properties of diesel fuel and especially of natural gas allow toe use of higher compression ratios (in comparison with gasoline engines) in diesel engines and gas diesel engines and thus ensure their high economic efficiency. However, very high compression ratios in certain conditions (for example, in forced operation modes) can result in hard engine operation, reduction of its economy and motor resources, and in some cases, destruction of a number of engine parts, for example [49]. In our opinion, the cause of the hard work of diesel engines and gas diesel engines is the self-ignition of local volumes of unburned mixture at the final stage of the combustion process. The statement of this problem [50-52] and its preliminary analysis show that the criterion of the form (21) in which the parameter t_f represents the characteristic burn-up time of the charge (diesel fuel torch and frontal combustion of gas fuel) is the main criterion of the problem under consideration.

As already noted, the dynamic problems listed above and the corresponding criterion relations do not exhaust all combinations of physical processes and corresponding characteristic times possible in the theory of combustion and explosion. To take at least a pre-chamber ignition engine, the mathematical model of the main process in which (for combustion of a mixture in chambers with allowance for the intercamera interaction of the combustion and discharge processes) was first developed by us [41, 53, 54]. In this problem characteristic times are: frontal combustion t_f (2), inter-chamber discharge of mixture (5) and piston motion t_m (6). In addition, in the special formulation of the problem of the prechamber engine, the characteristic times of convective heat transfer t_α (4), the bulk chemical reaction t_V (1), and others can also appear.

Conclusions

1) An attempt is made to classify the dynamic problems of the theory of combustion and explosion, the most famous of which are the problems of the classical theory of thermal explosion.

2) Classification of dynamic problems was carried out on the basis of an analysis of the relationships of six characteristic times of physicochemical processes in problems of combustion theory.

3) Theoretical analysis of dynamic problems shows that in the combustion theory there are at least 6 similarity criteria characterizing the competition of the characteristic times of various physical and chemical processes and a group of criteria of a combined type (in which there are at least three characteristic times and, correspondingly, at least two dynamic similarity criteria).

4) Analysis of the problems of the theory of combustion and explosion, as follows from the classical problems of the theory of thermal explosion and the dynamical problems considered above, shows that at the limit (that is, for critical values of dynamic variables (pressure p^*, temperature T^*, etc.), the solution is a criterial equation (complex dynamic similarity criterion) constructed from the characteristic times at the beginning of the process and the dynamic variables of the problem at the limit (index "*").

5) The dynamic similarity criterion or the corresponding criterion of the combined type obtained as a result of the solution of the problem is close to unity in order of magnitude (for example, equal to $\mathrm{e} = 2.718...$or $1/\mathrm{e}$).

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