dynamic viscosity; α, parameter characterizing the injection rate; η, ξ, similarity variables; a, parameter characterizing the thickness of the body; p_x, τ_x, F_x, projection, onto the symmetry axis, of the pressure and friction forces and the total force, referred to $\rho_\infty v_\infty^2$; q_x, heat flux to body surface; c_i, mass concentration of the i-th component of the mixture; M_i, molecular weight of the i-th component; γ, ratio of specific heats at constant pressure and constant volume; c, constant characterizing the pressure on the body surface (c = 1 according to Newton's theory); k, constant for the similarity problem $J(\eta) = \int_0^\eta F(h)d\eta$; $F(h) = p/\rho$; h, specific enthalpy, referred to u_∞^2; T_0, stagnation temperature; c_p, specific heat at constant pressure. Indices: δ, edge of boundary layer; w, surface of body; ∞, hypersonic flow; i, i-th component of mixture.

LITERATURE CITED

1. V. V. Lunev, "Similarity case of hypersonic flow of an imperfect heat-carrying gas about an axisymmetric body," Prikl. Mat. Mekh., 24, No. 3, 548-550 (1960).
2. W. H. Dorrance, Hypersonic Flows of an Imperfect Gas [Russian translation], Mir, Moscow (1966).

DYNAMICS OF GAS COMBUSTION IN A SPHERICAL VESSEL

V. I. Vodyanik

UDC 536.46

Equations are obtained to describe the dynamics of motion of a flame front and a gas in a spherical vessel. The possibility of a transition from combustion to thermal shock is demonstrated.

The combustion of a gas in a spherical vessel with central ignition is the simplest and most frequently theoretically and empirically studied case of combustion with a constant volume. The spherical vessel is often used as a convenient tool to determine the normal rate of propagation of a flame, maximum blast pressure, rate of increase in blast pressure, and certain other parameters of the process which are important for the solution of practical problems of industrial explosion-proofing. Nevertheless, the dynamics of flame propagation in a spherical vessel have yet to be described analytically. The literature [1, 2] contains theoretical descriptions of the dynamics of the pressure increase with an explosion. These descriptions employ differential equations requiring numerical solution on a computer.

As is known, the propagation of a flame in a gas is defined by its normal velocity u and the velocity of the burning gas. The character of the motion of the flame in a closed vessel is complicated by the fact that the velocity of the gas ahead of the flame is variable. However, it can easily be determined on the basis of the condition that the gases formed in front of the flame expand in the direction of the fresh gas and in the direction of the combustion products in a ratio which is proportional to the volumes of fresh gas and combustion products, respectively, at the given moment of time. This condition essentially follows from the condition of equality of the pressures at all points of the vessel during combustion.

A volume udt of fresh gas burns over an infinitesimally short interval of time dt on a unit surface of the flame. If the degree of increase in the volume of the gas with combustion is designated as ε, then the burned gas will occupy the volume εudt and the increment in volume will be $(\varepsilon - 1)$udt. It is this increment that is distributed proportionately as described above. In particular, in the case of a spherical vessel (Fig. 1), the following volume of gas is moved in the direction of the fresh gas

$$\frac{\frac{4}{3}\pi(R^3 - r^3)}{\frac{4}{3}\pi R^3}(\varepsilon - 1)\,udt.$$

All-Union Scientific-Research Institute of Safety Engineering of the Chemical Industry, Sverdlovsk. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 42, No. 5, pp. 750-757, May, 1982. Original article submitted March 31, 1981.

0022-0841/82/4205-0513$07.50

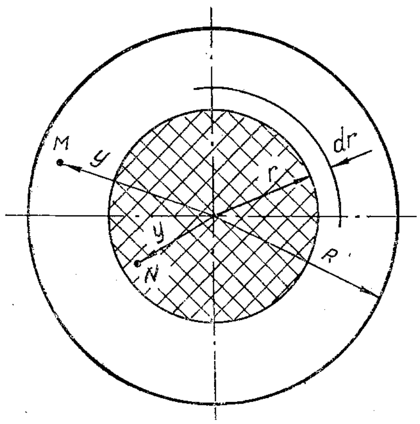

Fig. 1. Scheme of flame propagation in a spherical vessel.

This displacement also determines the motion of the fresh gas directly ahead of the flame front. Then the increase in the radius of the flame may be expressed as (Fig. 1):

$$dr = udt + \left(1 - \frac{r^3}{R^3}\right)(\varepsilon - 1)\, udt. \tag{1}$$

If in a first approximation we assume that u and ε are constant and are independent of the thermodynamic parameters of the gas in the vessel (which change during combustion) and if we introduce the notation $x = r/R$ and $a = \sqrt[3]{\varepsilon/(\varepsilon - 1)}$ then we can write the solution of differential equation (1) in the form

$$t = \frac{R}{u}\,\frac{a}{3\varepsilon}\left[\sqrt{3}\,\mathrm{arc\,tg}\,\frac{x\sqrt{3}}{2a - x} - \frac{1}{2}\ln\frac{(x-a)^2}{x^2 + ax + a^2}\right]. \tag{2}$$

In this equation, it is already taken into account that the integration constant is zero as a result of the initial conditions $t = 0$ and $x = 0$.

Equation (2) describes the displacement x of the flame front over time. The fact that this relation is expressed in explicit form relative to t rather than x makes it quite convenient to use, since the range of x is always the same and is $0 \leqslant x \leqslant 1$.

Figure 2 shows the dependence of the dimensionless complex

$$\lambda = \frac{a}{3\varepsilon}\left[\sqrt{3}\,\mathrm{arc\,tg}\,\frac{x\sqrt{3}}{2a - x} - \frac{1}{2}\ln\frac{(x-a)^2}{x^2 + ax + a^2}\right]$$

on the dimensionless displacement x of the flame front at different ε.

The dynamics of flame movement in a spherical vessel as described by Eq. (2) agree well with numerous experimental results [1]. We can obtain the apparent velocity of the flame directly from Eq. (1)

$$\frac{dr}{dt} = u\left[\varepsilon - (\varepsilon - 1)\frac{r^3}{R^3}\right], \tag{3}$$

from which it follows, in particular, that $dr/dt = \varepsilon u$ at the beginning of combustion at $r = 0$, that this velocity is slightly dependent on r, and that $dr/dt = u$ at the end of the process at $r = R$. Equation (3) can be conveniently used to analyze film scans of flame motion to empirically determine normal velocity. Here, not only can the initial section be used for the analysis – as is currently done – but the entire scan can be employed. Moreover, analysis of the results of such experiments using Eq. (3) reveals changes in u during combustion in a closed vessel due to changes in pressure and temperature.

If we set $x = 1$ in Eq. (2), we may express the total time of development of the explosion in the spherical vessel. This quantity is of great practical importance in explosion-proofing problems, so highly approximate empirical formulas – those in [3], in particular – are normally used for its calculation. It is recommended that it be determined from the condition that the ratio of the maximum rate of pressure increase to the mean be roughly equal to three, or that the mean apparent velocity of the flame in the spherical vessel be roughly four times greater than the normal velocity [4].

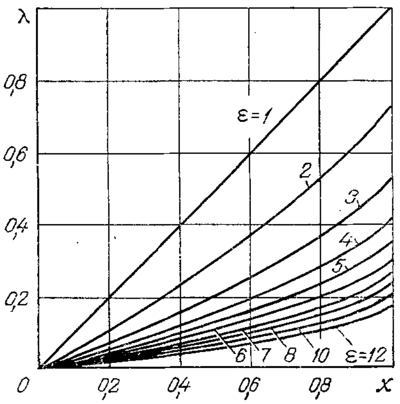

Fig. 2. Dependence of the dimensionless complex λ on the dimensionless displacement of the flame x at different ε.

The propagation of the flame in the vessel causes the fuel gas and combustion products to move. With a known law of flame front displacement, the gas motion problem can be solved graphically or numerically [5]. However, Eq. (2) allows us to solve it analytically.

To analytically describe the dependence of the displacement of an arbitrary point M (an infinitesimal volume of the fuel gas) on the displacement of the flame front (see Fig. 1), we write the condition of conservation of mass of the gas in the vessel during combustion:

$$\frac{4}{3}\pi r^3\rho_e + \frac{4}{3}\pi(R^3 - r^3)\rho = \frac{4}{3}\pi R^3\rho_0, \tag{4}$$

where ρ_e, ρ, and ρ_0 are running values of the densities of the combustion products and fuel gas and the initial density of the gas, respectively. Here, the spatial nonuniformity of the densities of the gases due to heat losses and the Mach effect will be ignored.

If we divide both sides of Eq. (4) by ρ and consider that

$$\frac{\rho_e}{\rho} = \frac{1}{\varepsilon} \text{ and } \frac{\rho_0}{\rho} = \frac{\frac{4}{3}\pi(R^3 - y^3)}{\frac{4}{3}\pi(R^3 - y_0^3)},$$

where y_0 is the initial position of the point M (before ignition of the mixture), we obtain

$$y = \sqrt[3]{y_0^3 + x^3\frac{\varepsilon - 1}{\varepsilon}(R^3 - y_0^3)}. \tag{5}$$

When solved simultaneously, Eqs. (5) and (2) describe the displacement of an arbitrarily chosen element of the fuel gas over time.

To describe the movement of an arbitrary point N (see Fig. 1) in the combustion products, both sides of Eq. (4) are divided by ρ_e. Here, it should be noted that by the end of combustion, point N, with the running coordinate y, occupies the initial position with the coordinate y_0. The density of the combustion products here will be ρ_0. Then

$$\frac{\rho_0}{\rho_e} = \frac{4}{3}\pi y^3 \Big/ \frac{4}{3}\pi y_0^3.$$

Thus, from (4) we can obtain an equation connecting the running coordinate of an element of the combustion products with the position of the flame front:

$$y = y_0\sqrt[3]{x^3 + \varepsilon(1 - x^3)}. \tag{6}$$

Equation (6), together with (2), describes the displacement of a volume element of the combustion products over time. As an example, Fig. 3 shows the displacement of the flame front according to Eq. (2) and an element of the gas according to (5) and (6) for different initial positions of the gas y_0.

Analysis of the dynamics of motion of the gases shows that the fuel mixture has a nonuniform acceleration field, with acceleration of the gas being significantly greater near the center of the vessel than at the periphery. The role of a strong and nonuniform acceleration field in a vessel may be quite substantial, for example, in the combustion of gas-disperse systems. This is because the acceleration field will result in different laws of displacement of the gaseous dispersion medium and the solid or liquid disperse phase, which will in turn inevitably lead to disturbance of the initial distribution of the concentration of the medium in the volume.

It is apparent from Fig. 3 that the gas velocity changes suddenly at the flame front. Analysis of the laws of motion of the fuel gas and combustion products under any conditions, such as in an open space, in a tube at the open or closed end, and in closed vessels of any shape, shows that the sudden change in gas velocity at the flame front is always the same and is equal to $\Delta v = u(\varepsilon - 1)$. This change in velocity evidently always occurs over distances equal to the thickness of the front. If in a first approximation we consider the motion of the gas at the front to be equally accelerated, then we may write the following for the acceleration ω:

$$\omega = \frac{\Delta v}{\Delta t} = \frac{u(\varepsilon - 1)}{\Delta t}.$$

On the other hand, we express the thickness of the flame front δ as follows:

$$\delta = u\Delta t + \frac{\omega(\Delta t)^2}{2}.$$

If the last two equations are solved simultaneously, excluding the time interval Δt from them, we obtain

$$\omega = \frac{u^2(\varepsilon^2 - 1)}{2\delta}. \tag{7}$$

By the thickness of the flame front, we mean the length of the heating and chemical reaction zones, i.e. the length of the zones in which the thermodynamic parameters of the gas change. If we take $\varepsilon = 6$, $u = 0.4$ m/sec, and $\delta = 0.5$ mm to evaluate the order of magnitude of the gas acceleration at the front, we obtain $\omega = 5600$ m/sec^2. Such a strong gas acceleration field at the flame front may lead to stratification of the intermediate and final combustion products of the reaction with respect to density, particularly if there is a solid phase such as soot among them.

All of the above conclusions are valid for the case where u is constant. However, it is well known that the normal velocity depends on the temperature and pressure of the fuel gas. These relations were expressed in [6] with exponential empirical formulas. In particular, for an adiabatic combustion process, it is recommended that the change in normal velocity be expressed by the formula [2]

$$u = u_0 \left(\frac{p}{p_0}\right)^{m+n-\frac{m}{\gamma}},$$

where u_0 is the normal velocity of the flame with the initial state parameters of the fuel gas; p and p_0 are the current and initial pressure of the gas.

However, such an exponential dependence of u on temperature agrees satisfactorily with experimental results at relatively low temperatures. The discrepancy becomes fairly large at temperatures close to the temperature of spontaneous combustion. Moreover, this relation can be used to determine values of u at temperatures above the spontaneous combustion temperature, which is physically contradictory. In connection with this, the author of [3] proposed that the dependence of normal velocity on the temperature T of the fuel gas be expressed by the following empirical formula:

$$u = u_n \frac{\ln\left(1 - \frac{T}{T_{sc}}\right)}{\ln\left(1 - \frac{T_n}{T_{sc}}\right)}, \tag{8}$$

where T_{sc} is the spontaneous combustion temperature; $T_n \approx 300$°K is the normal room temperature at which the handbook value of normal velocity of the flame u_n is determined.

Comparison of Eq. (8) with the well-known exponential relation at $m \approx 1.5$ shows that they

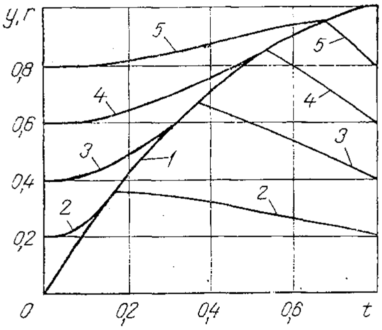

Fig. 3.

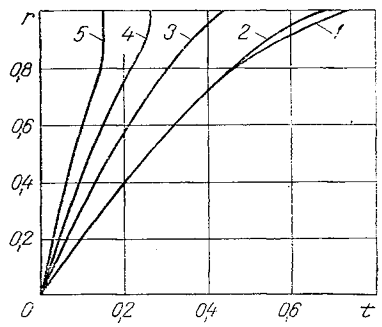

Fig. 4.

Fig. 3. Displacement of flame front according to Eq. (2) and of gas according to Eqs. (5) and (6) in a spherical vessel with R = 1 m at u = 0.4 m/sec, $\varepsilon = 6$; 1) flame front displacement; 2-5) displacement of gas element with its initial position relative to the center of the vessel corresponding to a distance $y_0 = 0.2$; 0.4; 0.6; 0.8 m. t, sec; y, r, m.

Fig. 4. Displacement of flame front in a spherical vessel with R = 1 at u = 0.4 m/sec, $\varepsilon = 6$, $p_0 = 0.1$ MPa, $p_b = 0.8$ MPa, $T_{sc} = 800°K$, $\gamma = 1.4$, $n = -0.2$; 1) according to Eq. (2); 2, 3, 4, 5) according to Eqs. (10) and (11), respectively, at $T_0 = 300$; 400; 500; 600°K.

give nearly the same values of u at temperatures significantly below T_{sc}. The advantages of Eq. (8) are seen at high temperatures and consist of the fact that $u \to \infty$ at $T \to T_{sc}$, i.e., the phenomenon of spontaneous combustion is described by Eq. (8) as the propagation of the front at an infinite velocity. This agrees well with the physical representation of the spontaneous combustion process as the combustion of the mixture simultaneously over the entire volume. The value of u cannot be determined if $T > T_{sc}$ is substituted into Eq. (8), which is another important advantage of this formula.

Thus, with adiabatic compression of the mixture during combustion, it is recommended that the change in u be expressed by the relation

$$u = u_n \left(\frac{p}{p_n}\right)^n \frac{\ln\left[1 - \frac{T_0}{T_{sc}}\left(\frac{p}{p_0}\right)^{\frac{\gamma-1}{\gamma}}\right]}{\ln\left(1 - \frac{T_n}{T_{sc}}\right)}, \tag{9}$$

where P_n is the normal (atmospheric) pressure at which u_n is determined.

Substitution of (9) into differential equation (1) yields

$$\frac{dr}{dt} = u_n\left[1 + \left(1 - \frac{r^3}{R^3}\right)(\varepsilon - 1)\right]\left(\frac{p}{p_n}\right)^n \frac{\ln\left[1 - \frac{T_0}{T_{sc}}\left(\frac{p}{p_0}\right)^{\frac{\gamma-1}{\gamma}}\right]}{\ln\left(1 - \frac{T_n}{T_{sc}}\right)}. \tag{10}$$

The running value of pressure in the spherical vessel may be related to the radius of the flame using the well-known formula [1]

$$\frac{r}{R} = \left[1 - \frac{p_b - p}{p_b - p_0}\left(\frac{p}{p_0}\right)^{-\frac{1}{\gamma}}\right]^{\frac{1}{3}}, \tag{11}$$

where P_b is the maximum final pressure with complete combustion of the mixture. Equations (10) and (11) constitute a system and can be solved simultaneously by numerical methods. As an example, Fig. 4 shows solutions of these equations for certain specific values of the mixture parameters. These solutions indicate that accounting for the dependence of u on temperature and pressure at temperatures considerably below the spontaneous combustion temperature yields a small correction to the results obtained with Eq. (2). The difference increases with temperature, and at

$$T_0 > T_{sc} \left(\frac{p_b}{p_0}\right)^{\frac{1-\gamma}{\gamma}}$$

the deflagration process changes over at a certain stage to spontaneous combustion. This is described by system (10), (11) as the attainment of a combustion rate equal to infinity.

Equation (11), together with (2) or (10), can also be used to describe the dynamics of the pressure increase with gas combustion in a spherical vessel.

In experiments, the phenomenon of spontaneous combustion of part of the volume of a mixture during its burning may be perceived as a transition to detonation, but there are important differences between the two: in detonation, the mixture is ignited as a result of shock compression in accordance with the Hugoniot curve; in the present case, the mixture is ignited as a result of compression in accordance with the Poisson curve; detonation propagates in the form of a wave with a certain finite velocity, while the process of spontaneous combustion described here occurs simultaneously in a certain volume of the fuel gas.

The above analytical solution of the problem of the transition of deflagrative combustion to spontaneous combustion does not take into account the duration of the induction period of the spontaneous combustion process, which, as is known, depends on the temperature of the mixture. Allowing for this time, spontaneous combustion should begin at a certain degree of "overcompression" of the mixture. However, obtaining an analytical solution for the thus-stated problem would require obtaining the dependence of the duration of the induction period on the thermodynamic paramters of the fuel mixture.

NOTATION

u, normal velocity of flame; t, time; π = 3.14159...; R, inside radius of spherical vessel; r, running radius of the spherical flame; ε, degree of expansion of the gas with combustion; x, dimensionless running radius of spherical flame; α, λ, dimensionless complexes; ρ, density of the gas; y, position of arbitrary point of gas relative to center of vessel; Δv, sudden change in gas velocity at flame front; ω, acceleration of gas; δ, thickness of flame front; m, n, temperature and barometric exponents; γ, exponent of adiabatic curve; p, pressure of gas; T, temperature of gas. Indices: 0, initial state; b, final state; e, combustion products; n, normal external conditions; sc, conditions of spontaneous combustion.

LITERATURE CITED

1. A. I. Rozlovskii, Scientific Principles of Explosion-Proofing in Work with Combustible Gases and Vapors [in Russian], Khimiya, Moscow (1972).
2. V. S. Babkin, V. I. Babushok, and L. G. Mikhailova, "Effect of thermodynamic and kinetic parameters on the dynamics of gas combustion in a spherical vessel," Fiz. Goreniya Vzryva, No. 6, 14-20 (1979).
3. V. I. Vodyanik, Explosion-Proofing Industrial Equipment [in Russian], Tekhnika, Kiev (1979).
4. É. A. Granovskii, V. N. Gudkovich, L. V. Novikova, L. I. Nuzhda, and L. P. Sidorenko, Methods of Calculating the Explosion- and Fire-Hazard Parameters of Gas and Dust-Gas Mixtures [in Russian], VNIITBKhP (All-Union Scientific Research Institute of Safety Engineering of the Chemical Industry), Severodonetsk (1975).
5. A. M. Garforth and C. J. Rallis, "Gas movement during flame propagation in a constant volume bomb," Acta Astonautica, 3, 879-888 (1976).
6. P. K. Senachin and V. S. Babkin, "On the 'knocking' effect in the combustion of gas in closed volumes," in: Combustibility of Materials and Chemical Agents for Fire-Extinguishing [in Russian], VNIIPO, No. 6, 7-9 (1979).