

Modelling of the gas combustion process

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This paper reports on a procedure which leads to the assessment of the K_G values without the need of determining the maximal rate of pressure rise by experiments. A simulation is proposed of the combustion process in its simplest form, i.e. one-dimensional propagation of the flame. Such simulation enables the burning velocity S_u to be assessed. Knowing the S_u values for different compositions of the flammable mixture makes it possible to determine the $S_{u,max}$ value. Once the correlation between $S_{u,max}$ and K_G has been established, this will enable us to assign an appropriate value of K_G to that of the maximal burning velocity. An example of such a correlation is given. It refers to flammable mixtures of a comparatively low burning velocity.

Keywords: flammable gas, burning velocity, rate of pressure rise, deflagration index K_G .

INTRODUCTION

The combustion of a flammable gas (flammable liquid vapours)-oxidizer mixture may vary in dynamics, depending on the type of the flammable gas, the type and the content of the oxidizing agent, the volume of the vessel used, and on some other factors. The dynamics of combustion (and this includes explosive combustion as well) can be described in terms of burning velocity¹ and, in a way, can also be regarded as a violence measure for the combustion process, including explosion. Burning velocity reaches maximal values, predominantly with the mixtures where the concentration of the flammable gas is slightly higher than the stoichiometric one. When oxygen content in the mixture is reduced, this is concomitant with a decrease in burning velocity (and consequently in the violence of explosion) to an extent, which depends on the type of the inert gas used for the purpose of dilution.

The parameters characterizing the violence of explosive combustion are determined experimentally via the measurements in a closed reactor. A recent Polish standard² recommends the use of an at least 0.005 m³ volume vessel, spherical or cylindrical in shape, with a unit enabling the measurements of initial pressure and explosion pressure with an accuracy of 0.05 bar and a time resolution of 1 ms. The procedures of both the mixture combustion and the pressure-time curve recording have to be carried out five times for each composition of the gas. Experimental determination of the parameters describing the combustion dynamics of a given gas requires a high-strength apparatus made of special, high-quality materials and equipped with the high-tech measuring and recording devices. The measurements, as well as the interpretation of the results obtained, are time-consuming (the reactor has to be dried and made subject to evacuation of impurities; the measurements must be repeated for the same composition; the measured curves require smoothing).

The $P = f(t)$ curves are used to determine the highest pressure, which is the explosion pressure P_{ex} , and the highest value of the derivative $(dP/dt)_{ex}$, which describes the rate of pressure rise. The plots of Fig. 1 depict an example of time-dependent variations in pressure and pressure derivative for a methane-air mixture.

The P_{ex} and $(dP/dt)_{ex}$ values are determined for different concentrations of the flammable gas in the oxidizer within the whole explosion range, from lower to upper explosion limits. And in this way the maximal values of the explosion pressure,

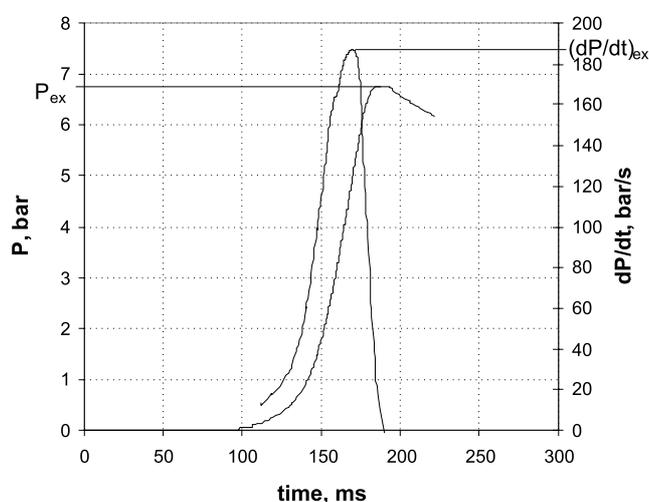


Figure 1. Variations in pressure P and in the rate of pressure rise, dP/dt , during the combustion of a mixture with 9.8 vol. % content of methane in air

P_{max} , and those of the rate of pressure rise, $(dP/dt)_{max}$, are obtained. The $(dP/dt)_{max}$ value depends on the volume of the experimental reactor. Thus, when determined in a 1 m³ reactor under quiescent conditions, it is denoted by the K_G symbol. When determined in a reactor of a different volume and thereafter converted into the K_G quantity according to the equation^{2, 6}:

$$K_G = \left(\frac{dP}{dt} \right)_{max} V^{1/3} \quad (1)$$

It is regarded as a constant that is independent of the reactor size and, therefore, suitable for characterizing a flammable substance (i.e. as a material constant). In a way, the K_G parameter is a 'guiding' indicator of the violence of explosion for a given gas in air. In engineering, the K_G value calculated in terms of equation (1) remains constant within a rather narrow range of volume variability of the reactor where the maximal rate of the rise in pressure is determined².

The burning velocity for a given mixture can be determined by experiments or assessed by computational methods³. Various experimental methods are available for the determination of the S_u values. As for the case of explosive combustion (in a reactor or, generally speaking, a closed space) reported on in this paper, it is possible to assess burning velocities in terms of the aforementioned rate of pressure rise (dP/dt) , i.e. the

quantity used for establishing the K_G value⁴. As opposed to equation (1), the procedure made use of for the determination of the burning velocity includes not only the reactor volume (as was the case with the K_G 'constant') but also (though to a smaller extent) such quantities that characterize the physical chemistry of the combustion process. In the present study we used this method to determine the experimental value of the burning velocity S_u . Using the experimental $(dP/dt)_{\max}$ value enables the attainment of the maximal burning velocity value $S_{u,\max}$. Seemingly, the $S_{u,\max}$ value may be regarded as a certain measure for the violence of explosion.

At the present state of the recognition of the problem, physical chemistry is taken into account when modeling the combustion process. To determine the burning velocity by modeling, use can be made of the professional CHEMKIN program, which has much to offer. Including a base of transport data (diffusion, heat conduction) and thermochemical data (enthalpies of components, specific heat, equilibrium constants), the program enables, for example, the simulation of a one-dimensional flame (subprogram PREMIX). For the purpose of computation, it is convenient to use balance equations for the continuity of mass, conservation of energy, and continuity of the components, as well as the equations of state⁵. Kinetics is described by a set of assumed elementary reactions and rate constants of these reactions in the given direction. As a result of the computations, we obtain the concentration variation profiles for particular reagents, the flame temperature profile and the burning velocity value.

In our considerations, all the factors associated with the random motion or (to express it in a more general way) the turbulence of the flammable mixture are neglected.

DETERMINING THE RATE OF EXPLOSION PRESSURE RISE

Pressure variations during the combustion of the methane-air-inert mixture were measured in a 20 dm³ spherical reactor with central ignition. A simplified diagram of the laboratory setup is shown in Fig. 2.

Assessing the K_G 'constant'

Measurements had been carried out at the initial pressure $P_0 = 1$ bar. From the pressure change during the combustion of a flammable mixture the value of $(dP/dt)_{\text{ex}}$ was determined. From the derived quantity and the size of the reactor ($R=0.168$ m), appointed for different compositions of the flammable mixture, the value of $(dP/dt)_{\max}$ was determined, and then K_G was calculated from the equation (1). The received average values of the K_G index were listed in Table 1.

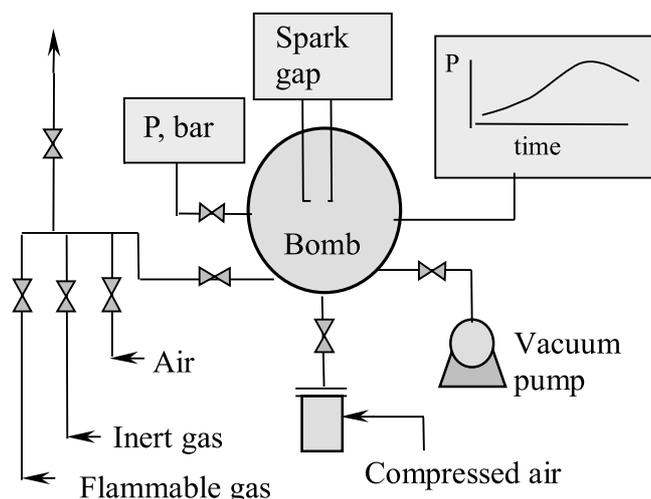


Figure 2. The apparatus for determining the explosion pressure and the rate of pressure rise

The maximal K_G value reported by Bartknecht for a quiescent methane-air mixture amounts to 55 bar·m/s⁶. Relevant Polish standard² recommends that the measuring apparatus (i.e. the size of the reactor and the energy of ignition) should be checked. The apparatus is regarded as suitable for the assessment of K_G , if the K_G value attained in a 20 dm³ reactor for a mixture of 10 vol. % CH₄ equals 65 bar·m/s. The K_G values reported on by other investigators for a methane-air mixture in a reactor of the same volume vary from 55 to 75 bar·m/s^{7,8}. The highest K_G value (75 bar·m/s) has been achieved for a mixture with no humidity.

Assessing the burning velocity value S_u

The recorded pressure-time curves were also used to calculate the S_u values according to the following equation⁴:

$$S_u = \frac{1}{3} R \frac{1}{P_{\text{ex}} (1+P)^{\frac{1}{\gamma_u}}} \left(1 - \left(1 - \frac{P}{P_{\text{ex}}} \right) \left(\frac{1}{P+1} \right)^{\frac{1}{\gamma_u}} \right)^{\frac{2}{3}} \frac{dP}{dt} \quad (2)$$

where R denotes the reactor radius, P indicates the actual pressure (above atmospheric), P_{ex} is the explosion pressure (the highest in the pressure variation plot) and γ_u stands for the heat capacity ratio, c_p/c_v .

The relation of (2) has been derived for an initial pressure of 1 bar. The results obtained for the methane-air mixture, together with the experimental values of pressure and pressure rise rate, like in Table 1, and with the γ_u value (which is 1.36), calculated in the point of curve inflexion $P(t)$, are plotted in Table 2.

The maximal S_u value for a mixture of 9.8 vol. % methane in air amounts to 45 cm/s. The experimental S_u values reported in the literature fall in the range 29 – 46 cm/s^{7,8}.

Table 1. The measurement values: the explosion pressure P_{ex} (above atmospheric) and derivative $(dP/dt)_{\text{ex}}$ in the inflexion point of the curve with pressure P ; the temperature 20°C

Lp	CH ₄ , % obj.	P_{ex} , bar	P , bar	$(dP/dt)_{\text{ex}}$, bar/s	K_G , bar·m/s
1	5.7	2.15	0.6	5.3	1.4
2	7.8	5.3	3.4	78	21.2
3	8.8	6.1	4.25	130.4	35.4
4	9.8	6.8	4.8	187.2	50.8
5	10.0	6.8	4.9	187.4	50.9
6	10.6	6.5	4.35	171.6	46.6
7	11.5	5.9	3.65	103.3	28.0
8	12.0	5.9	3.75	78.3	21.2
9	12.6	3.0	2.6	5.4	1.5
10	13.2	2.85	1.05	2.5	0.7

Table 2. Burning velocity S_u according to the formula (2), the derivative of burning velocity $(dS_u/dt)_{ex}$ according the formula (3) and the proportionality factor in the relation (3a)

Lp	CH ₄ , % obj.	S_u , cm/s	$-(dS_u/dt)_{ex}$, cm/s ²	K_G , bar·m/s	$-(dS_u/dt)_{ex}/S_u^2$, m ⁻¹
1	5.7	7.9	51.4	1.4	82.3
2	7.8	30.3	544.8	21.2	59.3
3	8.8	37.4	900.0	35.4	64.4
4	9.8	45.0	1377.2	50.8	68.0
5	10.0	44.0	1317.0	50.9	68.0
6	10.6	44.3	1370.0	46.6	69.8
7	11.5	29.6	656.0	28.0	74.9
8	12.0	25.6	418.9	21.2	63.9
9	12.6	4.0	6.5	1.5	40.9
10	13.2	3.9	7.02	0.7	46.0

A certain similarity between values S_u and K_G can be noticed. This similarity has been analysed in the aspect of quantitative relations.

The relation (2) can be written in the abbreviated form:

$$S_u = \frac{1}{3} R f(P) g(P) \frac{dP}{dt} \quad (2a)$$

where a denotation was made:

$$f(P) = \frac{1}{P_{ex} (1+P)^{\frac{1}{\gamma_u}}}, \quad g(P) = \left(1 - \left(1 - \frac{P}{P_{ex}} \right) \left(\frac{1}{1+P} \right)^{\frac{1}{\gamma_u}} \right)^{\frac{2}{3}}$$

The relation (2) can be next rewritten in the form:

$$S_u = \left(\frac{1}{36\pi} \right)^{\frac{1}{3}} f(P) g(P) \left(\frac{4\pi}{3} \right)^{\frac{1}{3}} R \frac{dP}{dt} = \left(\frac{1}{36\pi} \right)^{\frac{1}{3}} f(P) g(P) K_G \quad (2b)$$

In this notation proportionality between S_u and K_G values appears.

Quantities of the $f(P)$ function with the dimension of pressure converse as well as the nondimensional one $g(P)$ are dependent on the ultimate pressure P_{ex} and pressure P in the inflexion point of the $P(t)$. If it is the curve of functions f and g (for pressure accompanying the highest values of combustion rate – points 4, 5, 6 in Tables 1 and 2), are equal adequately: 0.0401 bar⁻¹ and 1.0558. The total factor of proportionality between the S_u and K_G values is about 0.0088. Therefore, the formula (2b) takes the form:

$$S_u = 0.0088 K_G \quad (2c)$$

This formula refers to the mixtures with the nearly stoichiometric composition from the rich mixture side.

For propane, that factor under similar conditions is 0.0081.

The burning velocity derivative (acceleration – deceleration of combustion), calculated in the inflexion point of the curve $P(t)$, is shown by the relation received from formula (2):

$$\frac{dS_u}{dt} = -S_u \frac{1}{\gamma_u (1+P)} \left(1 + \frac{2}{3} \frac{\gamma_u (1+P) + (P_{ex} - P)}{P_{ex} (1+P)^{\frac{1}{\gamma_u}} - (P_{ex} - P)} \right) \frac{dP}{dt} \quad (3)$$

It can be rewritten in the form:

$$\begin{aligned} \frac{dS_u}{dt} &= -S_u^2 \frac{3}{R \gamma_u (1+P) f(P) g(P)} \left(1 + \frac{2}{3} \frac{\gamma_u (1+P) + (P_{ex} - P)}{P_{ex} (1+P)^{\frac{1}{\gamma_u}} - (P_{ex} - P)} \right) \\ &= -S_u^2 \frac{3}{R \gamma_u (1+P) f(P) g(P)} h(P) \end{aligned} \quad (3a)$$

The accepted above values of functions $f(P)$ and $g(P)$ are 0.0401 bar⁻¹ and 1.0558, the estimated value of $h(P)$ function is equal to about 1.286 (the average pressure value for the measurement points is 4.85 bar of overpressure in the inflec-

tion point). The total factor of proportionality in the equation (3a) is then about 68 m⁻¹ or

$$\frac{dS_u}{dt} = -68 S_u^2 \quad (3b)$$

For propane this factor is 78.8 m⁻¹.

There appear to be analogies between the quantities S_u and K_G . Seemingly, the two quantities are interchangeable with each other, so they can be used in this way when we attempt to characterize the violence of the combustion process. The correlation depicted in Fig. 3 offers evidence to suggest such approach. It shows how the burning velocity S_u calculated from the pressure plot and the explosion index K_G determined for various methane-air-inert (N₂, Ar, CO₂) mixtures are interrelated.

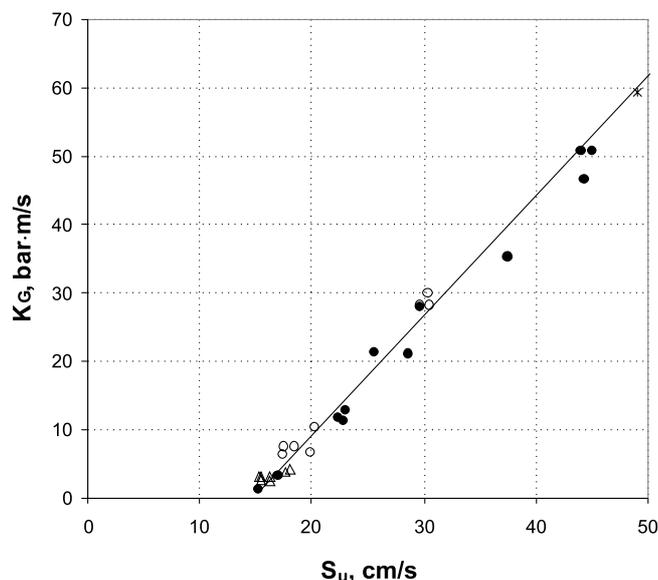


Figure 3. The experimental value of K_G related to the S_u value calculated from the $P=f(t)$ plot for the following mixtures: • – CH₄-air-N₂; o – CH₄-air-Ar, Δ – CH₄-air-CO₂, * – C₃H₈-air

For a flammable mixture of a relatively low burning velocity it may be safely assumed that the S_u - K_G relation is approximately linear. The equation that describes this line:

$$K_G = 1.75 S_u - 25 \quad (3)$$

fairly well characterizes the relation in Fig. 3. Thus, if the above assumption also holds true for the mixtures displaying higher burning velocities, it will be possible to make use of the burning velocities, obtained by modelling the combustion process and assess the explosion index K_G on the basis of an appropriate $K_G = f(S_u)$ correlation. It is advisable to use the S_u value obtained by computational methods.

Computation of burning velocity

In the foregoing analysis, which aimed at assessing the burning velocity for methane-air mixture, we made use of the experimental rate of explosion pressure rise. Hence, we may classify the procedure as both an experimental and a computational one. Now, we can say that a procedure involving computations alone is becoming feasible; the burning velocity can be attained by the mathematical modelling of the combustion process. More specifically, if we consider a simplified, one-dimensional model of flame propagation, we are offered the possibility of attaining the parameter S_u by the sub-program PREMIX of the professional program CHEMKIN⁵. By making use of the program, we have been able to assess the burning velocity for the methane-air mixture and compare the S_u values obtained via the above route with those assessed using the experimental-computational procedure (Fig. 4). Our computations involved the mechanism underlying the combustion of hydrocarbons, which consists of 84 elementary reactions and has been proposed by Warnatz⁹.

The maximal burning velocity value, $S_{u,max}$, can be taken from the plot in Fig. 4. The substitution of this value into the relation of (4) leads to the assessment of the K_G value, which approaches 54. Fig. 4 also shows the S_u values obtained using the experimental-computational procedure.

A similar relation can be derived for any flammable mixture, initial pressure and initial temperature. The potential use of a relation similar to that of (3) necessitates the construction of one or several correlations between the explosion index and the burning velocity within a wide range of variability for both parameters.

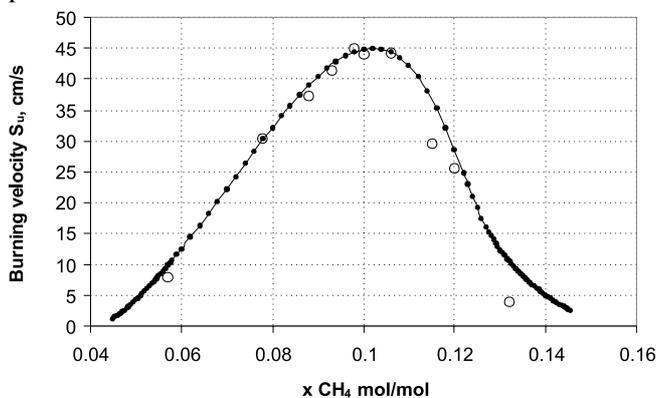


Figure 4. Burning velocity S_u vs composition of the methane-air mixture: • – the values calculated using the CHEMKIN program; o – values calculated from experimental $P=f(t)$ curves

SUMMARY

A procedure is outlined for the assessment of the explosion index, K_G , without referring to the maximal rate of pressure rise determined experimentally.

The experiments involved are time-consuming, and the result obtained is marked by the influence of the reactor volume and ignition energy. This is primarily due to the motion of the flammable mixture induced by the fuel and the reactor walls.

It is suggested that the experimental procedure (which is troublesome and not fully unequivocal in terms of the result obtained) should be substituted by the simulation of the combustion process in its simplest form: the one-dimensional propagation of the flame.

The simulation of the process carried out in this way leads to the assessment of burning velocity. Knowing the S_u values

for different compositions of the flammable mixture makes it possible to determine the $S_{u,max}$ values.

After establishing the correlation between $S_{u,max}$ and K_G , it will be possible to assign an appropriate value of K_G to that of $S_{u,max}$. Such a correlation has been established in this paper in order to exemplify the problem. The correlation is of a linear nature and refers to flammable mixtures of relatively low burning velocities, that is to say: mixtures of methane and air or mixtures of methane and air deficient in oxygen.

SYMBOLS

K_G	– explosion index, bar·m/s
P	– actual pressure, bar
P_{ex}	– explosion pressure, bar/s
$(dP/dt)_{ex}$	– rate of explosion pressure rise, bar/s
$(dP/dt)_{max}$	– maximum rate of explosion pressure rise, bar/s
R	– reactor radius, m
S_u	– burning velocity, m/s
$S_{u,max}$	– maximal burning velocity, m/s
dS_u/dt	– burning velocity derivative, m/s ²
V	– reactor volume, m ³
γ_v	– heat capacity ratio c_p/c_v

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