

Penetration of the laminar flames of natural gas–oxygen mixtures through conical obstacles

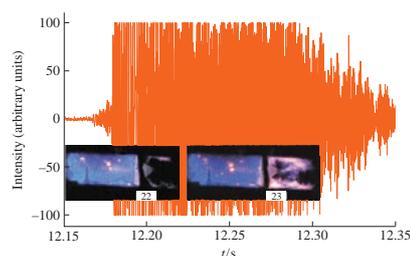
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It has been experimentally found that a flame of dilute natural gas–oxygen mixtures does not penetrate through the central opening of a confuser, but it penetrates only through the central opening of a diffuser, even if there are additional openings on the cone elements. The numerical modeling performed using compressible dimensionless reactive Navier–Stokes equations in a low Mach number approximation made it possible to qualitatively interpret the results.



The hazards of methane explosions and flame deflagrations still represent a threat for chemical plants, mining tunnels, pipes, etc. Accidental fires in process industries can cause enormous losses of human lives and capital.^{1–4} A challenge is to eliminate and reduce the consequences of accidental fires and explosions in pipes. To achieve that goal, accurate data concerning model setups are required to understand the characteristics of methane explosions in pipes⁵ and in production floor areas, combustion chambers and chemical reactors, which represent volumes of complex geometry. The modeling of turbulent premixed explosions involved in deflagrating flames inside a confined chamber remains a challenging problem particularly with respect to the adequate representation of the burning rate and the structure of the reaction zone.

In hazardous gas explosions typically found in process industries, the number and location of openings in obstacles are the parameters (along with the shape of an obstacle, blockage ratio, size, etc.) that affect the severity of such explosions.^{6,7} However, the influence of the parameters is poorly understood.

In low-speed turbulent combustion applications, the low Mach number approximation of reactive Navier–Stokes equations is an appropriate basis for a qualitative simulation.^{8,9} The heat release generated by combustion creates flow instabilities in the forms of buoyancy and gas expansion, which in turn intensifies a natural transition from laminar to turbulence. Turbulence also enhances combustion by increasing the mixing process. In our consideration, a premixed flame propagates first as a laminar spherical front wrinkled by obstacles and becomes a turbulent flame propagating at higher speeds.

We have earlier shown that the flame of a natural gas–oxygen mixture does not pass through a cone with the only opening in its center located as a confuser, but the flame readily penetrates through the diffuser. It means that, under the same conditions, the limit of penetration of dilute methane oxygen flame through a diffuser is markedly less than in the case of a confuser; therefore, the confuser is the most effective flame arrester.¹⁰ There are no published data on flame penetration through the cone with the

central opening if there are additional openings on the elements of the cone.

In addition, we have found that maximum pressure and maximum acoustic intensity are much greater for the plain obstacle with several openings as compared with that with a single opening.¹¹ The observed pattern is likely a reflection of the fact that two openings and more, especially three ones, are more effective turbulators than a single one.

In this work, we studied the flame propagation through the cone oriented both as a diffuser and as a confuser with round openings with additional ones on the elements of the cone. The numerical modeling of the observed regularities using compressible dimensionless reactive Navier–Stokes equations in a low Mach number approximation was performed.

We also considered the means of improving the models taking into account relative contributions of gas dynamic and chemical factors in combustion, which can be used for the simulation of flame propagation through the obstacles of different geometry.

The experiments were performed with stoichiometric methane–oxygen mixtures diluted with CO₂ and Ar (the reagents of chemically pure grade) at initial pressures of 100–200 Torr and an initial temperature of 298 K in a horizontal cylindrical quartz reactor 70 cm in length and 14 cm in diameter. A pair of spark ignition electrodes was located at the butt-end of the reactor. The reactor was fixed in two stainless steel gateways at butt-ends, supplied with inlets for gas pumping and gas inflow and a safety shutter, which swung outward when the total pressure in the reactor exceeded 1 atm.^{9–13} Plastic funnels ($d = 14$ cm) with a central opening and two openings (17 mm in diameter each) on the elements of the cone [the opening angles of the funnels were 55° and 83° (Figure 1)] were oriented both as a diffuser and a confuser and placed at the center of the reactor. The obstacle was fixed in the reactor with a foam ring (see Figure 1). The combustible mixture (15.4% CH₄ + 30.8% O₂ + 46% CO₂ + 7.8% Ar) was prepared (CO₂ was added to decrease a flame front velocity and to enhance the quality of filming, Ar was added to diminish the discharge threshold); the dependence of the phenomena



Figure 1 Conical obstacle with three openings (opening angle, 83°).

observed on the equivalence ratio of the mixture needs separate investigation. The reactor was filled with the mixture up to a necessary pressure. Then, spark initiation was performed (the discharge energy was 3 J). The speed filming of ignition dynamics and flame front (FF) propagation was carried out from the side of the reactor^{9–13} with a Casio Exilim F1 Pro color high-speed digital camera (frame frequency, 600 s^{-1}). Simultaneous detection of radicals CH ($A^1\Delta-X^2\Pi$) at 431 nm ¹⁴ was carried out with the use of the second Casio Exilim F1 Pro high-speed movie camera equipped with a $430 \pm 15\text{ nm}$ interference filter (40% transmittance at 430 nm). A video file was stored in computer memory and its time-lapse processing was performed. The pressure change in the course of combustion was recorded by a piezoelectric gage synchronized with the discharge. Acoustic oscillations were recorded with a Ritmix sensitive (up to 40 kHz) microphone. The audio file was stored in computer memory and analyzed with the Spectra Plus 5.0 software package.

The representative experiments of high-speed filming of FF propagation in the combustible mixture at an initial pressure of 165 Torr through the cone obstacle oriented as a confuser and as a diffuser are shown in Figure 2 for the cone opening angles of 55° and 83° . Under our conditions, flame always penetrated only through the central opening of the diffuser. At the same time, the flame penetrated only through lateral openings of the confuser at the cone opening angle of 55° [Figure 2(a), frames 21, 22; Figure 2(c), frame 19]. In this case, the combustion was accompanied by a loud and sharp sound and the shutter swings outward. Note that flame propagation under conditions of diffuser is not accompanied by a sharp sound effect, and the shutter does not swing. Figure 3 shows the time dependences of acoustic amplitude for flame propagation, illustrating the aforesaid, in the reactor containing the confuser [Figure 3(a)] and the diffuser [Figure 3(b)].

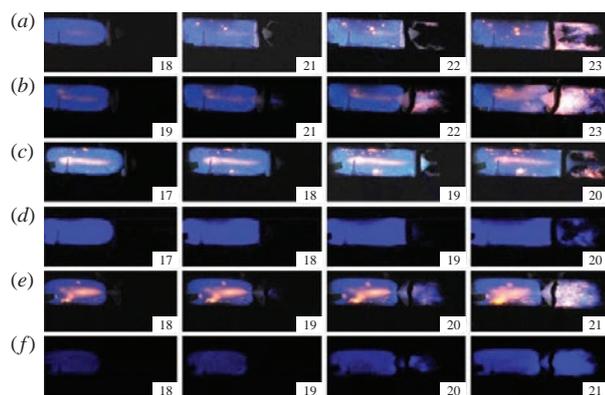


Figure 2 High-speed filming of FF propagation through the cone obstacle with a central opening and two openings on the elements of the cone: (a) a confuser (cone opening angle, 55°); (b) a diffuser (cone opening angle, 55°); (c) a confuser (cone opening angle, 83°); (d) a confuser (cone opening angle, 83°), a 430 nm interference filter is placed before the camera; (e) a diffuser (cone opening angle, 83°); (f) a diffuser (cone opening angle, 83°), a 430 nm interference filter is placed before the camera. Initial pressure, 165 Torr. The figures on each frame correspond to the frame number after initiating discharge.

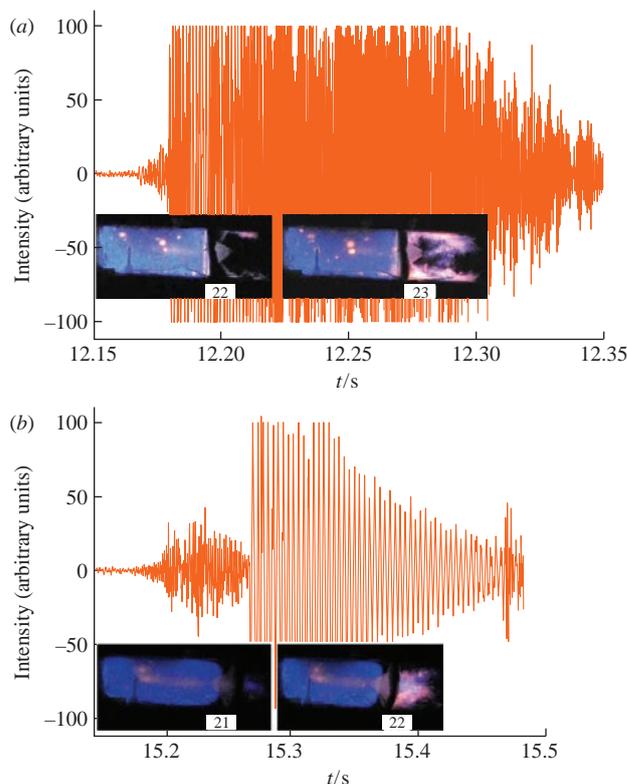


Figure 3 The time dependence of acoustic perturbation amplitudes at flame propagation in the gas mixture at an initial pressure of 165 Torr. (a) Confuser, corresponding frames from Figure 2(a) are shown, the center of each frame corresponds to the current time; (b) diffuser, corresponding frames from Figure 2(b) are shown, the center of each frame corresponds to the current time.

With an increase in the opening angle, the flame begins to penetrate through the central opening of the cone [Figure 2(c), frames 19, 20]. The opening diameters in the conic obstacle are significantly smaller than the minimum diameter of flame penetration through a plain obstacle with a single central opening (20 mm^{11}). Therefore, in assessing the fire safety of a room or confinement with several openings, the minimum size of the single opening should not be used because, with an increase in the number of openings, the diameter of the opening sufficient for flame penetration decreases.

In case of a plain obstacle with three openings (the opening angle is obviously 180°), the flame penetrates through each of the three openings at the same time.¹¹ In our case, a conic cavity influences the development of combustion by the occurrence of reflected acoustic waves with stagnant zones and the interaction of these waves with the initial combustion front, which has generated waves; maximum pressure is thus implemented at some distance from cone top.¹⁵ The complexity of the process provides, in particular, the observed feature that with decreasing the opening angle in the obstacle with a central opening at a certain value of this angle the flame does not penetrate through the opening at all¹⁰ regardless of the existence of additional openings on the elements of the cone.

Conversely, with an increase in the opening angle in the obstacle, its shape tends towards the plain one, at which the flame penetrates through each of the three openings at the same time;¹¹ therefore, at a certain value of this angle, the flame will penetrate through all openings. This is shown in Figures 2(c) and 4(b).

Numerical modeling based on compressible dimensionless reactive Navier–Stokes equations in a low Mach number approximation,⁸ which describe flame propagation in a two-dimensional channel^{16,17} showed a qualitative consent with experiments.^{9–13}

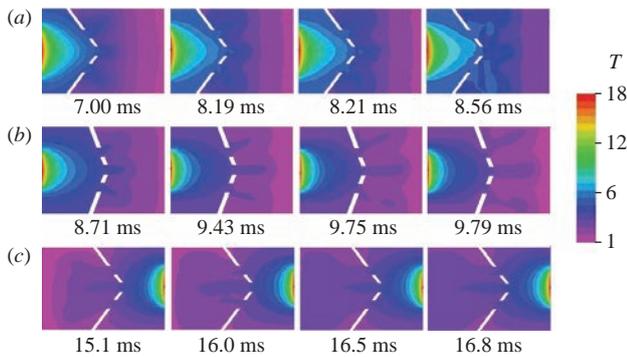


Figure 4 Qualitative calculation of flame penetration through the conic obstacle. Change in dimensionless temperature for flame propagation through (a) a confuser for the single Arrhenius reaction, the opening angle of the diffuser is 100° ; (b) a confuser for the single Arrhenius reaction, the opening angle of the diffuser is 150° ; (c) a diffuser for the single Arrhenius reaction, the opening angle of the diffuser is 100° . The scale of dimensionless temperature is presented on the right.

The problem was solved by finite element analysis with the FlexPDE 6.08 package.¹⁸ Initiation condition was taken as $T = 10$ on the boundary of the channel; there was a conical obstacle with two additional openings on the elements of the cone in the center of the channel. Boundary conditions (including the obstacle) were $C_x = 0$, $C_y = 0$, $n = 0$, $u = 0$, $v = 0$, $\rho_x = 0$, $\rho_y = 0$, and convective heat exchange $T_t = T - T_0$. A chemical reaction was presented by a single first-order Arrhenius equation.

The results of qualitative calculations of flame penetration through the conic obstacle as both the confuser and diffuser are shown in Figure 4. The calculations are in qualitative consent with the experiments shown in Figure 2; namely, the flame penetrates through the diffuser [Figure 4(c)] and does not propagate through a central opening of the confuser [Figure 4(a)] with the smaller opening angle (100°). At the larger opening angle [150° , Figure 4(b)], the flame penetrates through all the three openings in the confuser in qualitative agreement with experimental data (see Figure 2). In the case of a plain obstacle with three openings (one of them is a central one, and the opening angle is 180°), the flame penetrates through each of the three openings.¹¹ Evidently, the qualitative consideration (a single Arrhenius reaction instead of a complete chemical mechanism, two-dimensional modeling, etc.) does not allow one to obtain the angle at which the flame begins to penetrate through the central opening of the confuser. In addition, such a qualitative difference from the process of flame penetration through a plain obstacle with the central opening indicates a noticeable role of interaction of acoustic fluctuations in the reactor containing a conic obstacle with the propagating front of combustion even for subsonic flames.

Therefore, regardless of the qualitative consideration, we took into account the main features of flame propagation through a conic obstacle with additional openings on the cone elements. Namely, the flame does not penetrate through the central opening

of the confuser, but it penetrates only through that of the diffuser even if there are additional openings on the elements of the conic obstacle.

Note that the analysis of a three-dimensional model is necessary for the quantitative description of the flame penetration through a conic obstacle. At the same time, the results of the two-dimensional modeling are in qualitative agreement with experimental data. In addition, the results obtained by the visualization of flame penetration through orifices of different shape are important for the solution of explosion safety problems for volumes of complex geometry such as production floor areas, combustion chambers and chemical reactors.

References

- 1 S. Kundu, J. Zanganeh and B. J. Moghtaderi, *J. Loss Prev. Process Ind.*, 2016, **40**, 507.
- 2 B. Zhang, L. Pang and Y. Gao, *Fuel*, 2016, **168**, 27.
- 3 B. J. Lowesmith, G. Hankinson and D. M. Johnson, *Process Saf. Environ. Prot.*, 2011, **89**, 234.
- 4 A. Pekalski, J. Puttock and S. Chynoweth, *J. Loss Prev. Process Ind.*, 2015, **36**, 365.
- 5 F. Lees, *Lees' Loss Prevention in the Process Industries: Hazard Identification, Assessment and Control*, 4th edn., Butterworth-Heinemann, 2012.
- 6 S. R. Gubba, S. S. Ibrahim, W. Malatasekera and A. R. Masri, *Combust. Sci. Technol.*, 2008, **180**, 1936.
- 7 J. Kindracki, A. Kobiera, G. Rarata and P. Wolanski, *J. Loss Prev. Process Ind.*, 2007, **20**, 551.
- 8 V. Akkerman, V. Bychkov, A. Petchenko and L.-E. Eriksson, *Combust. Flame*, 2006, **145**, 675.
- 9 N. M. Rubtsov, *The Modes of Gaseous Combustion*, Springer, 2016.
- 10 N. M. Rubtsov, I. M. Naboko, B. S. Seplyarskii, V. I. Chernysh, G. I. Tsvetkov and K. Ya. Troshin, *Mendelev Commun.*, 2016, **26**, 61.
- 11 N. M. Rubtsov, V. I. Chernysh, G. I. Tsvetkov and K. Ya. Troshin, *Mendelev Commun.*, 2018, **28**, 99.
- 12 N. M. Rubtsov, V. I. Chernysh, G. I. Tsvetkov and K. Ya. Troshin, *Mendelev Commun.*, 2017, **27**, 101.
- 13 N. M. Rubtsov, A. N. Vinogradov, A. P. Kalinin, A. I. Rodionov, K. Ya. Troshin, G. I. Tsvetkov and V. I. Chernysh, *Mendelev Commun.*, 2017, **27**, 192.
- 14 B. Lewis and G. von Elbe, *Combustion, Flames and Explosions of Gases*, 3rd edn., Academic Press, New York, London, 1987.
- 15 O. V. Achasov, S. A. Labuda, V. V. Kondrashov, O. G. Penyaz'kov, R. M. Pushkin, A. I. Tarasov and S. I. Shabunya, *J. Eng. Phys. Thermophys.*, 1993, **65**, 1073 (*Inzhenerno-Fiz. Zh.*, 1993, **65**, 548).
- 16 A. Majda, *Equations for Low Mach Number Combustion*, Center of Pure and Applied Mathematics, University of California, Berkeley, 1982, report no. 112.
- 17 F. Nicoud, *J. Comput. Phys.*, 2000, **158**, 71.
- 18 G. Backstrom, *Simple Fields of Physics by Finite Element Analysis*, GB Publishing, Malmö, Sweden, 2005.

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