On the Nature of the Acoustic Oscillations in Gas Explosions

Iurii Kh. Polandov¹, Anton Korolchenko¹ and Sergei Dobrikov²

¹Moscow State University of Civil Engineering, Yaroslavskoe shosse, 26, Moscow, Russia
²MERA (Nizhniy Novgorod, Russia)

E-mail: ikbs@mgsu.ru

Abstract. The possible existence of acoustic oscillations (oscillating combustion) in gas explosions in unclosed volumes is known. A significant increase in risks was confirmed, if it happens indoors, which makes studies in this direction relevant. But the solution to this problem has proven difficult for two reasons. First, the results of the experimental studies turned out to be reproducible with weak reliability. This circumstance takes place, despite the fact that the first classical experiments, resulting in acoustic oscillations during gas heating, date back to the 19th century. The second reason why research is difficult is that by now there are no reliable mathematical models describing the process of excitation and development of oscillating combustion in gas explosions. The gas explosion simulation using the example of cylindrical chamber with a diameter of 200 mm and a length of 1.5 meters and a window on the lateral surface. The chamber in the initial state is filled with propane-air mixture, which is ignited at the left end along the chamber axis. The validity of mathematical model was checked by comparing the results of the gas explosion development calculation in the tube with other known results obtained in the closed circular tubes.

1. Introduction

The possible existence of acoustic oscillations (oscillating combustion) in gas explosions in unclosed volumes is known. A significant increase in risks was confirmed, if it happens indoors, which makes studies in this direction relevant. [1, 2, 3]. But the solution to this problem has proven difficult for two reasons. First, the results of the experimental studies turned out to be reproducible with weak reliability [4]. This circumstance takes place, despite the fact that the first classical experiments, resulting in acoustic oscillations during gas heating, date back to the 19th century [5]. This event was designated as a phenomenon and named as the “singing” Higgins flame in honor of the author who discovered it. "Singing" occurred in a long vertical tube, open at both ends, when the burner was ignited inside the tube in its lower quarter. The burner and flame position was stationary. Experiments of Rijke, who heated the air in a similar tube, not by a flame, but an electric coil are also known. According to Raushenbach B.V. research [5] the reason for the excitation of such oscillations is the existence of zones of varying viscous friction along the tube. It is noteworthy that the oscillation frequency in these devices is determined by the first natural frequency in the tube-air system. The reproducibility of these experiments is good.

There are many similarities between classical experiments and explosion experiments, among which the main sign of generality is gas heating and its oscillations at the acoustic frequency. Classical experiments of course are the foundation for understanding the processes occurring during oscillating combustion, but there are also serious obvious differences between the two types of experiments.
Among the latter, it should be noted the different process time: in explosion, it is fast, and in “singing” experiments it is stationary (quasistationary). In addition, in the classical version, the position of the gas heating unit in the tube is stable, and in explosions the position of flame front is variable in space and time. And, indeed, the geometry of units with acoustic oscillations is different. These and other differences in the development of processes make it impossible to determine the nature of excitation and development of oscillations in explosions, their prediction and, most importantly, their prevention. Use the version of the excitation of oscillations due to the chamber wall friction is also not possible, since the main hydraulic losses in explosion in chambers occur in the window narrowing, and not on walls, as in classical experiments.

The second reason why research is difficult is that by now there are no reliable mathematical models describing the process of excitation and development of oscillating combustion in gas explosions. Naturally, this refers to models based on the methods of computerized fluid dynamics, CFD, because lumped parameter models, in principle, prove unequal to this task. The FLACS and ANSYS programs widespread in Europe do not include in the list of solvable problems the excitation of acoustic oscillations in the explosion [6, 7, 8, 9]. The results of simulation of gas explosions in open volumes carried out in the USA are of greater interest [9, 10], in the first case by a numerical method using the OpenFOAM program based on Large Eddy Simulation (LES), and in the second case - by a numerical method by Xu S. et al. and by semianalytic method. In both cases, equations describing linearized oscillatory circuits were included in the system of the basic laws of gas dynamics for an ideal gas, written in the Euler form. In the first case, this is the oscillations of chamber boundaries, and in the second case, the oscillations of gas column in the chamber. In the analytic method, the solution was represented as a Fourier series, although without taking into account the Gibbs effect.

It is clear that such studies shed light on the mechanics of excitation of acoustic oscillations, but so far they offer no grounds for predicting the oscillating combustion in open volumes.

2. Research objective

The possibilities of numerical methods for solving a system of equations describing the basic laws of gas dynamics are disproportionately wider than any other methods. It is clear that the mathematical models of gas explosions are based on the same equations, but differ from each other in the methods of solution, specific nature of posed problems, gas properties, boundary conditions, and other features. In this paper, Vulkan-M software product was used in solving [12, 13], based on the Large-Particle Method (LPM) developed by Belotserkovsky O. M. and Davydov Yu. M. [14]. The LPM is based on dividing the calculated volume into a large number of “particle” cells (usually about 100 thousand), in each of which the basic laws of gas dynamics in the form of the Euler equations (or Navier-Stokes) are fulfilled, and at the boundaries of each particle, the parameters are “joined”. By virtue of the fact that this method has the inherent conservatism of the solution at the level of each particle, in solving conservatism remains valid throughout the calculated space.

The flame propagation is described inside the particle, the front velocity is composed of the flow velocity and normal combustion rate, which results in burnout only part of the mixture in the particle. The flame spreads to other particles in the presence of unburnt gas mixture. The fraction of burnt gas mass is used to calculate the supply of thermal energy in the particle and take this into account in the energy conservation equation. The system is closed by the ideal gas law in the form of Clapeyron equation.

The solution of simultaneous equations is carried out according to the explicit scheme; therefore, the requirement for particle size and time steps is reduced to the fulfillment of the Courant-Friedrichs-Levy criterion. In our case, it turned out that the input of equations describing the flame propagation impairs the stability of solution, so the criterion value had to be decreased by more than two orders to ensure the computational stability.
Taking into account the fact that the system solution does not require a preconceived idea of the way of system solution, and the method of calculation uses minimal computational resources as compared to others, the use of Vulcan-M software in calculation of gas explosions, including in case of possible oscillating combustion is of scientific and practical interest.

3. Mathematical model

General Provisions

The gas explosion simulation using the example of cylindrical chamber with a diameter of 200 mm and a length of 1.5 meters and a window on the lateral surface. The chamber in the initial state is filled with propane-air mixture, which is ignited at the left end along the chamber axis. The following assumptions regarding the simulated environment were made:

– initial mixture is homogeneous and stoichiometric;
– physical characteristics of the initial mixture, combustion products and air are the same;
– gases and their mixture involved in the physical process are inviscid and ideal;
– burning runs in particles located at the boundary between the unburnt mixture and combustion products;
– window opens immediately after the excess pressure in the chamber and remains open throughout the entire experiment;
– action of gravity is neglected;

The particles have the cube shape of 1 cm on edge, thus forming an “Eulerian mesh” in the calculated space. The time step was $5 \times 10^{-7}$ s, which ensures the value of count stability criterion during the whole experiment not more than $1.5 \times 10^{-2}$ s. The calculation consists of the repetition of time steps. In turn, each such step includes three stages:

1) "Eulerian", in which all the effects associated with the gas movement are neglected (there is no mass transport across the boundaries of cells); on the fixed Eulerian mesh, the intermediate values of the required flow parameters are determined;
2) "Lagrangian", in which the mass flow motion through the boundaries of "Eulerian" cells is simulated and they are redistributed in space. It is assumed that the entire mass is transferred only due to the velocity component normal to the boundary;
3) final, in which the final values of flow parameters based on the laws of conservation of mass, pulse and energy for each cell and the system as a whole are determined.

The system structure includes the heat and mass exchanging processes with the environment and flame propagation. The cooling-down processes on the chamber walls are estimated on the basis of data obtained in pressure decay physical experiments in the closed chamber explosion. To calculate the outflow through open boundary, the pressure in the cell at the boundary is taken to be equal to the average between the pressure values in the cells from the chamber and atmospheric pressure. Different colors were used for particles that simulate real objects in the process visualization: boundaries, window flow area, flame front and gases. The Bezier method was used in tracing gas flow; they are black in the figures. The temperature of gases in the tube is reflected by a change in the emissivity of cells, with temperature growth the cells become lighter.

System of equations

The gas dynamics equations are written in a scalar version
\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{U}) &= 0 \\
\frac{\partial \rho U_x}{\partial t} + \text{div}(\rho U_x \vec{U}) &= 0 \\
\frac{\partial \rho U_y}{\partial t} + \text{div}(\rho U_y \vec{U}) &= 0 \\
\frac{\partial \rho U_z}{\partial t} + \text{div}(\rho U_z \vec{U}) &= 0 \\
\frac{\partial \rho E}{\partial t} + \text{div}(E \rho \vec{U}) + \text{div}(p \vec{U}) &= 0
\end{align*}
\]

where \( \rho \) – density, kg/m\(^3\);
\( U_x, U_y, U_z \) – velocity vector components in x, y and z direction, m/s;
\( \rho \) – pressure, Pa;
\( E \) – specific total energy,
\[
E = I + \frac{U^2}{2}
\]
where \( I \) – specific internal energy, J/kg;
The system is complemented by the ideal gas law
\[
p = \rho I (\gamma - 1)
\]
where \( I \) – specific internal energy, J/kg;
\( \gamma \) — adiabatic exponent of the medium.

This system of equations is open due to the uncertainty of \( E \) value. During the finite-difference approximation elaboration, the \( \Delta E \) value is determined using the equations describing the flame propagation.

**Consideration of the flame front propagation process**

In order to describe the flame propagation process, an approach that fits organically into the approximation system model is used, and according to which an additional cell condition parameter – the mass fraction of combustion products \( f \) in the cell is entered. This parameter for each cell can be expressed as follows:
\[
f = \frac{m_B}{m}
\]

where \( m \) – total mass of the mixture in the cell, kg;
\( m_B \) – mass of combustion products in the cell, kg.

In this case, the computational cells are divided into three groups (with the calculation errors – \( \epsilon \)):
– cells with the initial mixture for which the condition is fulfilled \( f < \epsilon \);
– "burnt-out" cells – \( f > 1 - \epsilon \);
– "burning" cells \( \epsilon < f < 1 - \epsilon \).

A complete model description and difference schemes used are presented in [4].

Simulation of the combustion process is carried out in three steps. In the first step, gas combustion in the cells is considered. For all "burning" cells, the fraction of gas \( \Delta f \), that burned during time \( \Delta t \) is determined, and energy \( \Delta E \) release is calculated:
\[
\Delta f = \frac{\Delta t}{\Delta t} U_B
\]
\[
f_i = f + \Delta f
\]
\[
\Delta m = \Delta f \cdot m
\]
\[
\Delta E = \Delta m H
\]
\[ E_v = mE + \Delta E = mE + \Delta mH \]  
\[ \Delta l – \text{cell edge length, m;} \]
\[ E_p – \text{specific total energy of the mixture in the cell, J/kg,} \]
\[ \Delta E – \text{energy release, J,} \]
\[ H – \text{calorific power of the mixture, J/kg.} \]

For 3D cells of a regular mesh, the characteristic linear size is the cube edge length \( \Delta l = \Delta x = \Delta y = \Delta z \). 
In this paper, the power dependence of normal burning rate vs. change in the mixture temperature is assumed. [15]:

\[ U_n = U_{nv} \left( \frac{T}{T_{nv}} \right)^\beta \]  
\[ \text{where } \]
\[ U_{nv} – \text{normal flame propagation velocity in a stationary mixture under normal conditions, m/s,} \]
\[ T \text{ and } T_{nv} – \text{current mixture temperature and mixture temperature under normal conditions, respectively, K,} \]
\[ \beta – \text{power dependence factor.} \]

\[ T = \frac{p\mu}{\rho R} \]  
\[ \text{where } \mu – \text{molar mixture mass, kg/mol,} \]
\[ R – \text{absolute gas constant, J/(K*mol).} \]

The second simulation step is the fire propagation to neighboring cells. The first and second steps assume the immobility of medium, which is typical for the "Eulerian" stage of the computational cycle of large-particle method [1].

The third step is to take into account the burnt gas mass transfer across the cell boundaries (final stage of the large particle method). The transfer is simulated similarly to the transfer of other parameters. However, due to the specific nature of \( f \) parameter, the use of the same expressions for determination of transferred values is inadequate. In this regard, the authors propose special calculation formulas for the transferred \( f \) values based on its physical interpretation.

General transfer formulas for \( f \) parameter:

\[ f_{i+1/2,j,k} = \begin{cases} 1, & (f_{i,j,k} > 1 - \varepsilon) \lor (f_{i+1,j,k} > 1 - \varepsilon) \\ 0, & (f_{i,j,k} < \varepsilon) \lor (f_{i+1,j,k} < \varepsilon) \\ f_{i,j,k} + f_{i+1,j,k} \end{cases} \]

(11)

Use of formula (11) to determine the transferred values of \( f \) parameter ensures the appropriate application of the general transfer formula for this parameter.

Expression (11) also makes it possible to determine the fire propagation conditions to neighboring cells (the second step of combustion simulation). The "ignition" condition of an “unburnt” cell \((i,j,k)\) from a cell\((i+1,j,k)\) is written as (12):

\[ f_{i+1/2,j,k} > \varepsilon \]  
(12)
4. **Mathematical model validity check**

The validity of mathematical model was checked by comparing the results of the gas explosion development calculation in the tube with geometrical dimensions described in Section 2, with other known results obtained in the closed circular tubes (without a window). Ignition was carried out at the left end. The front (Figure 1) repeats the forms that have become classical, in the first half of the tube they have an aspect of ellipsoid, and in the second - an aspect called “tulip” in publications. The pressure growth (Fig. 2a) also corresponds to the known curves. At the beginning it resembles a curve typical for central explosion in a spherical vessel, then, touching the cylinder walls, it sharply reduces the rate of pressure build-up. When the flame front took the form of a tulip, the pressure increases almost linearly. The numerical experiment provides the possibility to calculate also the flame front area, more precisely, the number of burning cells (Fig. 2 b). It is entirely consistent with the pressure profile.

At the beginning of the process, the front grows rapidly, then after touching the walls, it also decreases sharply, and after adopting the shape of a tulip, its area practically does not change, until it touches the right end, after which it decreases to zero.

5. **Gas explosion in the tube with side hole**

Let us assume that in the chamber described in section 2, there is a window on the lateral surface, which diameter varies from 60 mm to 62 mm. If assume that the window diameter is 60 mm (or 61 mm) and place it at a distance of 45 mm from the left tube end, then the explosion simulation shows that the intense pressure oscillations are set up in the tube (Figure 3). They set up at the moment when the flame front passes a window (Fig. 4) and intense gas (and flame front) oscillations begin at the center of tube (Fig. 5).
First one can pay attention to the fact that simultaneously with pressure oscillations and changes in the flame front area, oscillating gas velocities appear in the tube (Fig. 5), second, frequencies and the development nature of these values completely coincide (Fig. 3 and Fig. 5). Third, the pressure maximum amplitudes and velocity are delayed with respect to the maximum oscillating amplitude of the flame front. Oscillation frequencies synchronously increase over the course of time from 100 to 200 Hertz.

Figure 6 compares the pressure values on the left and right ends, it can be seen that they are opposite in phase, which means that acoustic waves develop in the tube, represented by a quarter of the wavelength, that is, the length is $L=1.5\times4=6$ m. The pressure beams are at the ends of the tube, and the speed beam is in the center of the tube (Fig. 6). Using known ratios the average temperature in the tube can be calculated: at the beginning of oscillations it is about 750 K and at the end of the process it is 1500 K, which is very likely to be true.

The amplitude of pressure oscillations in the window cells is much smaller than the amplitudes at the ends, but that should be the case, because the window is located between the pressure node and beam. But it is on the one hand. On the other hand, the flow in the window is associated with a drop in pressure compared to the pressure in the tube.
Figure 4. Visualization of the flame front spread in the tube with a window: 0.05 s – no oscillation; 0.1 s – beginning of oscillations; 0.13 s – intensive growth; 0.15 s – maximum amplitude of oscillation.

Figure 5. The dynamics of axial gas velocity in the center of the tube.

Figure 6. Pressure profile in different tube points during oscillations.
The influence of acoustic oscillations on the average pressure in the tube is clearly seen when estimating the difference between gas explosions without and with acoustic oscillations. With a slight difference between the diameter of windows 60, 61 and 62 mm, the explosion pressure charts look as shown in Fig. 7. It is apparent that the buildup of acoustic oscillations leads to the reduction in burst time, and consequently to the intensification of combustion and increase in the average explosion pressure.

![Figure 7](image)

**Figure 7.** The border existence of a stable "very loud" flame between the values of the tube diameter 61 mm and 62 mm.
1 – diameter 60 mm; 2 – diameter 61 mm; 3 – diameter 62 mm

6. Results and discussion

The coincidence of major characteristics of pressure oscillations, flame front area and axial gas velocity along the tube center, gives grounds to consider them directly interrelated. It can be assumed that the oscillatory gas motions along the tube axis (Fig. 4) “tousle” the front, while changing the number of burning cells and at the same time the reference area of the burning front (“turbulizing the flame”).

With regard to the facts that in the mathematical model we deal with an ideal gas and only gas dynamics equations are taken into account, which, as it is well known, describe well the propagation of acoustic and shock waves, we can definitely say that the oscillating circuit in the model is formed by these particular equations. The "feedback" mechanism in this oscillating circuit is based entirely on the assumed flame propagation model. This mechanism provides excitation, growth and damping of acoustic oscillations.

Such parameters as the window location and its dimensions, which, in general, does not contradict the well-known results of sound theory have impact on acoustic oscillations. With one difference: we are dealing there with a stationary or quasistationary process, and in our case it is clearly unsteady and fast.

The desire to call a gas explosion accompanied by acoustic oscillations, a “singing explosion” by analogy with the "singing Higgins flame", disappears, if we take into account the destructive force that is contained in this process.

The adopted mathematical model and its software "Vulcan M" with an acceptable level of visualization of the calculation results describe adequately a gas explosion in a cylindrical chamber.

References

[1] Gorev V. A., Belyaev V. V., Fedotov V. N. The condition of the beginning of vibration combustion in a depressurized rectangular vessel // Physics of combustion and explosion. – 1989 – Vol. 25, No. 1 Pp. 36-39.

[2] C. Regis Bauwens, Jeff Chaffee, Sergey Dorofeev. Effect of Instabilities and Acoustics on Pressure Generated in Vented Propane-Air Explosions. 22nd ICDERS July 27-31, 2009 Minsk, Belarus.

[3] C. Regis Bauwens, Sergey B. Dorofeev. Parameters Affecting Flame-Acoustic Flame
Instabilities Vented Explosions. 24th ICDERS July 28 - August 2, 2013 Taipei, Taiwan.

[4] I. H. Polandov, S. A. Dobrikov, D. A. Kukin. The results of the tests vent panel designs. Fire-explosion safety, No. 8 2017, Pp. 5 – 14. Russia

[5] Rauschenbach B. V. Vibracionnoe gorenie (Vibration burning). M.: Fizmatgiz, 1961. 500 s.

[6] Helene H. Pedersen, Prankul Middha. Modelling of Vented Gas Explosions in the CFD tool FLACS. A publication of AIDIC. The Italian Association of Chemical Engineering Online at: www.aidic.it/cet.

[7] Xu, S., Aslam, T., & Stewart, D. S. High resolution numerical simulation of ideal and non-ideal compressible reacting flows with embedded internal boundaries. Combustion Theory and Modelling, 1(1), 113-142. DOI: 10.1080/713665233.

[8] Yu. V. Zakharaeva, N. N. Fedorov. Simulation of explosion in a confined space using ANSYS AUTODYN. Institute of theoretical and applied mechanics to them. S. A. Khristianovich. Siberian branch of RAS, Novosibirsk, Russia

[9] Guoning Rao, Yun Zhang, Weiguo Cao, Mengke Zhao, Wei Gao, Hao Liang and Yinxing Tan. Experimental and Numerical Studies of Premixed Methane-Hydrogen/Air Mixtures Flame Propagation in Closed Duct. The Canadian Journal of Chemical Engineering, March 2018.

[10] Luc Bauwens, C. Regis L' and Ida Wierzba. Oscillating flames: Multiple-scale Analysis. Proceedings of Royal Society A.(2009) 465, 2089–2110/ doi:10.1098/rspa.2008.0388/ doi:10.1098/rspla.2008.0388

[11] C. Regis Bauwens, Jeff Chaffee, Sergey Dorofeev. Experimental and Numerical Study of Methane-air Deflagrations in a Vented Enclosure. Fire Safety Science–Proceedings of the 9 International Symposium, pp. 1043-1054. International Association for Fire Safety Science.

[12] Iurii H. Polandov and Sergei A. Dobrikov. Features gas explosion in a cylindrical tube with a hole on the side// INASE, New Developments in Pure and Applied Mathematics. The International Conference on Mathematical Methods, Mathematical Models and Simulation in Science and Engineering. Vienna, Austria, March 15-17, 2015.

[13] [Barg MA, Polandov Yu.H., Markov SS The certificate of the official registration of the computer program 2007614950 Simulation of the processes of combustion and explosion of gas mixtures "Vulkan-M"; applicant and copyright holder OrelSTU. - Application No. 2007613936; claimed. 08/10/2007; registered on 03.12.2007. – 1 p. (rus).

[14] O. Belotserkovskiy, M. Davydov. Metod krupnykh chastits v gazovoy dinamike (Method of large particles in gas dynamics). - Moskva: Nauka, 1982. – 370 p.

[15] Molkov V.V.. Dinamika sgoraniya gaza v negermetichnom sosude (Dynamics of combustion of gas in an unsealed vessel): Dissertatsiya kand. fiz.-mat. nauk: spets. 01.04.17 / - M., 1983. – 211 p.