Burning law determination using numerical simulation of propellants burning in the closed vessel

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Abstract. This paper proposes a method of determining the "real" combustion law based on numerical simulation that also takes into account the thermal transfer between the hot gases resulting from deflagration and the walls of the vessel. This method is validated using the experimental results obtained in the closed vessel for SB propellant type, used in small-caliber propulsion systems. The proposed method is implemented using Ansys Fluent software, having as input the properties of the closed vessel walls from technical literature and of the gases resulting from the deflagration of propellant, calculated using a thermochemical model. To simulate the burning phenomena of the propellant charge and the impact that may occur between the propellants elements, on the one hand, and between the propellants element and the inner walls of the vessel, on the other hand, we used a dynamic mesh and mathematical models using UDF. For validation we used the diagrams from experimental tests made in the closed vessel at two different loading densities, the results obtained being in good agreement with the experimental ones. Moreover, the method used allows us to evaluate the error due to not taking into account the thermal losses that occurred in the closed vessel.

1. Introduction

In order to design and develop new propulsion systems, the firing tests in the closed vessel are required. There are two types of vessels: closed and with gas leakage nozzle, being used to study the ballistic behaviour of propellants with applicability in both military and civilian fields. [1]

In propulsion systems, the propelling charge is transform by deflagration into gases whose energy manages to propel bullets, projectiles, rockets, fragments, etc. The deflagration of the propelling charge occurs at high pressures (1000-5000bar) and high temperatures (1500-3000K), the phenomenon taking place in a very short period of time (1 to 20ms). In order to determine the burning law of propellants, it is necessary to know their ballistic characteristics, characteristics that can be calculated through a series of tests at constant volume. There are a number of methodologies for determining the burning law of propellants using tests in the closed vessel, many of them based more or less on simplifying assumptions. The closest reality model is the one based on the physical law of
combustion of the powder. However, the existing models do not take into account the thermal transfer phenomena between the hot gases and the walls of the closed vessel. [1]

**Closed vessel,** figure 1 and figure 2, is a component part of the manometric installation. It consists of the following parts:
1. main body;
2. bolt for crusher (recorders);
3. ignition bolt;
4. pressure gauge;
5. exhausting device.

![Figure 1. Closed vessel.](image)

Figure 2 represent a cylindrical vessel open on both ends, with thick walls made of steel used to manufacture fire mechanisms. The inner space of the vessel forms in the middle part a cylindrical chamber, in which the quantity of the investigated powder is burned. At both ends of the chamber, there are slight outward-facing extensions for inserting the shutter rings. Both ends of the inner space of the vessel are threaded for screwing nuts: one for crushers and the other one for the primer. The outer side of the vessel has, on both sides, parallel faces for a better fixation of the vessel in the latch of the lathe during assembly and disassembly. [1]

**Bolt for crusher,** consists the closed vessel, inside which is the crusher, which deforms under the pressure of the gases. Outside, the nuts have a hexagonal head, with a longitudinal cut, the middle threaded and a projection on the frontal part. The lower part of this subassembly has a channel, in which the pistol well-adjusted moves and which transmits the gas pressure on the crusher, at the other end the crusher rests on the bottom of plug stop, screwed into the threaded hole of the hex head of the nut. [1]

**Ignition bolt** with a hexagonal head and a threshold at the front end, it has a coaxial channel which present a conical extension towards the head of the bolt; in the channel is inserted rod, electrically insulated from the bolt through an insulating membrane or cigarette sheet and which serves as an electric current conductor for primer’s ignition. [1]

The inner part of the rings is rotated according to a special profile and as a result, the outer surfaces of the rings under the pressure of the gases are well pressed by the walls of the vessel and by the ends of the nuts, which excludes the possibility of escaping the dust gases outside.

Regarding the preparation and execution of the experiments, the calculation and preparation of the loads of the research powder, the primer and the assembly of the vessel are included. [1]
There are different types of propellants like flake, ball, cord, single perf (tubular), ellipsoid. In this case the form that we used is flattened spherical powder, as you can see in figure 3. [2]

Burn rate determines how fast a propellant burn. The amount of propellant actually available for burning at that burn rate is determined by the shape of the propellant, mass and the grain geometry. The burning takes place at the surface in parallel layers from outside to inside as a function of pressure as is written in equation (1). [2]

\[
u = u_1 p^\eta \text{[m/s]} \tag{1}\]

where: \(u_1\) is the burn rate coefficient, \(p\) is the pressure and \(\eta\) is the pressure exponent.

Figure 2. Main components of the closed vessel.

Figure 3. Powder used in our experiments.
To initiate the burning of propellants it’s used a primer which weight is calculated for a pressure $p_a = 5 \times 10^6 \, \text{Pa}$ using the formula:

$$w_e = W_0 \left(1 - \frac{\Delta}{\delta} \right) \frac{p_a}{f_a + \alpha_a p_a}$$  \hspace{1cm} (2)

where:

$W_0[\text{cm}^3]$ - closed vessel’s volume

$\Delta [\text{g/cm}^3]$ - loading density

$\delta [\text{g/cm}^3]$ - powder’s density

$f_a [\text{J/kg}]$ - impetus

$\alpha_a [\text{cm}^2/\text{g}]$ - covolume

It is usually taken:

- for $\delta = 0.1-0.2 \, \text{g/cm}^3$
- for $\delta = 1.6 \, \text{g/cm}^3$

- for the primer of black powder $f_a = 900000 \, \text{J/kg}$, $\alpha_a = 0.5 \, \text{cm}^2/\text{g}$

2. Deduction of the profile of the powder elements with the flattened spherical shape according to the burned thickness

Flattened spherical shape can be approximated with a cylindrical form which parallel surfaces are elliptical. Equation of the ellipse in Cartesian coordinates is:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$  \hspace{1cm} (3)

In addition to this equation, we use the following equations necessary to deduce the profile of the powder element in the first quadrant [3]:

$$\frac{y_f - y_i}{x_f - x_i} = \tan \beta$$

$$\left( x_f - x_i \right)^2 + \left( y_f - y_i \right)^2 - a^2 = b^2$$  \hspace{1cm} (4)

To determine the profile of the element we need the positions $(x, y)$ corresponding to each point on the curve. These are determined by a fourth degree form equation $x^4 + a_1 x^3 + a_2 x^2 + a_3 x + a_4 = 0$ namely:

$$x_1^4 = x_1^2 x_2 - \frac{x_1^2 (a^4 - a^2 x_2^2 + b^2 x_2^2 - a^2 b^2)}{b^2 - a^2} x_1 \frac{2a^4 x_2 - a^4 x_2^2}{b^2 - a^2} = 0$$  \hspace{1cm} (5)

where $a_1 = -2a_2$, $a_2 = \left( \frac{a^4 - a^2 x_2^2 + b^2 x_2^2 - a^2 b^2}{b^2 - a^2} \right)$, $a_3 = -2a^4 x_2$, $a_4 = \frac{a^4 x_2}{b^2 - a^2}$

Making the substitution $w = \frac{a_1}{4} + x$, we determine the equation of degree 4 in which the coefficient of $w^3$ is 0: $w^4 + pw^2 + qw + r = 0$. This equation (6) is called the fourth degree reduced equation.

$$w^4 + w^2 \left( -\frac{3a_1^2}{8} + a_2 \right) + w \left( \frac{2a_1^3}{16} + \frac{a_1 a_2}{4} + a_3 \right) + \frac{-3a_1^4}{256} + \frac{a_2 a_4}{16} - \frac{a_1 a_3}{4} + a_4 = 0$$  \hspace{1cm} (6)
where: \( p = \frac{-3a_1^3}{u} + a_2 \), \( q = \frac{2a_1a_2}{u} + \frac{a_2^2}{4} + a_3 \) și \( r = \frac{-3a_1^6}{256} + \frac{a_2a_3^2}{16} - \frac{a_2^3a_4}{4} + a_4 \)

To solve this 4th degree equation we use René Descartes' method. It started from the idea that a polynomial of fourth degree can be written as a product of second polynomials of second degree [3], that is:

\[
w^4 + pw^3 + qw + r = (w^2 + aw + b)(w^2 + aw_1 + b_1)
\]

where \( a, a_1, b, b_1 \) must be determined.

By identifying the coefficients the system is obtained:

\[
\begin{align*}
\alpha + \alpha_1 &= 0 \\
b + b_1 + a\alpha_1 &= p \\
abla b_1 + a_1b &= q \\
b_1b &= r
\end{align*}
\]

(8)

The last equation can be written as follows:

\[
(b_2 + b)^2 - (b_1 - b)^2 = 4r
\]

(9)

There: \( \alpha_1 = -\alpha \), \( b_1 + b = p + a^2 \), \( b_1 - b = \frac{p}{a} \)

By replacing these relations in equation (7) we obtain:

\[
a^6 + 2pa^4 + (p^2 - 4r)a^2 - q^2 = 0
\]

(10)

Note \( a^2 = u \), we have the following equation:

\[
u^3 + 2pu^2 + (p^2 - 4r)u - q^2 = 0
\]

(11)

same as \( ax^3 + bx^2 + cx + d = 0 \) where \( a=1, b=2p, c=p^2 - 4r, d=-q^2 \)

The cubic polynomial \( \mathfrak{P}: \ ax^3 + bx^2 + cx + d = 0 \) has solutions:

\[
x_1 = S + T - b / 3a
\]

(12)

\[
x_2 = \frac{S + T}{2} - \frac{b}{3a} + \frac{i\sqrt{3}}{2}(S - T)
\]

(13)

\[
x_3 = \frac{S + T}{2} - \frac{b}{3a} - \frac{i\sqrt{3}}{2}(S - T)
\]

(14)

where:

\[
S = \sqrt[3]{R + \sqrt{Q^3 + R^2}}, \quad T = \sqrt[3]{R - \sqrt{Q^3 + R^2}}
\]

(15)

and in turn:

\[
Q = \frac{3ac - b^2}{9a^2}, \quad R = \frac{9abc - 27a^2d - 2b^3}{54a^3}
\]

(16)

So we find \( u \), that means \( a, a_1, b, b_2 \) so that the equation of fourth degree can be solved by extracting square roots.

We consider \( w_2, w_3, w_4 \) the roots of the equation \( w^4 + pw^3 + qw + r = 0 \).
Based on Viete's relations we obtain the 4 roots of the equation \( w^4 + pw^2 + qw + r = 0 \) with the expressions [3]:

\[
\begin{align*}
   w_1 &= \frac{1}{2} (\sqrt{u_1} + \sqrt{u_2} - \sqrt{u_3}) \\
   w_2 &= \frac{1}{2} (\sqrt{u_1} - \sqrt{u_2} + \sqrt{u_3}) \\
   w_3 &= \frac{1}{2} (\sqrt{u_1} + \sqrt{u_2} + \sqrt{u_3}) \\
   w_4 &= \frac{1}{2} (-\sqrt{u_1} - \sqrt{u_2} - \sqrt{u_3})
\end{align*}
\]  

(17)  
(18)  
(19)  
(20)

From these values we choose the relation (17) that meets the imposed requirements. Thus we can find the value of \( x_1 = \frac{w_1 + w_2}{2} \) and respectively the value of

\[
y_1 = y_2 = \frac{a^2 - x_1^2}{a^2 - x_1^2 - b^2} \sqrt{\frac{a}{a^2 - x_1^2} + b^2 x_1^2}
\]  

(21)

So we can find out the relation between \( y_2 \) și \( x_2 \) resulting:

\[
y_2 = -ad \frac{a^2 - x_1^2}{a^2 - x_1^2 + b^2 x_1^2} + \frac{b\sqrt{a^2 - x_1^2}}{a}
\]  

(22)

3. Numerical simulation

3.1 The physical model

The physical model of the working area is composed of the closed vessel, the tested powder and the primer, presented in the previous figures. The physical model is characterized by the properties of the materials that are in solid state (the powder elements) and which undergo combustion a phase transformation, the properties of the materials that are in a compressible fluid state (the combustion products and the air), as well as the solid material of which the body of the closed vessel is made, and although it does not directly influence the gasodynamic parameters, due to the fact that it allows the thermal transfer, reduces the energy of the powder gases formed. All these aspects of the real phenomenon are taken into account in the numerical modelling performed. [4]

The powder gases generated by the combustion of the flowing powder represent a complex mixture of chemical species, which due to temperature and pressure variations undergo dissociation, recombination, condensation, etc. In the simulated model it was considered that combustion generates a non-reactive gas from a chemical point of view whose properties have been theoretically determined by thermodynamic calculation as a function of temperature at various pressures. [4]

The numerical simulation model of powder deflagration in the 10 \( cm^3 \) closed vessel using the FLUENT program is based on the general equations of fluid mechanics and the real gas state equation, to which burning rate equation is attached to simulate the conditions of the powder elements and the primer on the mobile borders. [5]

The complexity and size of the system under consideration and the axial symmetry of certain component parts of the system make it possible to approach the problem of fluid mechanics in the 2D domain as an axial-symmetric problem on an equivalent model. The proposed equivalent model and the method of establishing equivalence are presented below. [5]
3.2 The equivalent physical model. Determining the equivalent combustion rate coefficient

The equivalent physical model of the 10 cm³ closed vessel in the two-dimensional case, used in numerical simulation is shown in figure 4 and figure 5.

The equivalent physical model made is based on the following considerations (equivalence conditions)[5]:

a) The volume of the closed vessel chamber of the equivalent model shall be the same as the actual one;

b) The physico-chemical properties of the equivalent powder and of the gas generated will be the same as in the real case;

c) In the simulated case, a single spherical powder element is used;

d) Mass of the powder and the mass of the primer in the proposed model must be the same as the mass of the powder and the mass of the actual primer;

e) The density of the equivalent powder is the same as the actual density;

f) The flow rate of combustion products on the powder element should be the same for both the equivalent powder and the real powder;

g) The fraction of powder burned from an element should be the same in both cases.

According to f) hypothesis, the law of burning rate of the powder is expressed by \( u = u_e \cdot p^V \).

Based on the equivalence conditions stated above and assuming that the exponent of the burn rate remains constant, it can be determined \( u_e \).

3.2.1 Determining the equivalent burning rate coefficient

a. The real powder

It consists of flattened spherical powder elements, which, after studying them under a microscope, can be approximated with cylindrical elements which section is elliptical. The dimensions for a real powder element are as follows:

1. Large diameter of the element: \( D = 1 \) mm;

2. Small diameter of the element: \( d = 0.8 \) mm;

3. Element height (combustion thickness): \( h = 0.3 \) mm;

4. Initial volume of the element \( V_0 = \frac{\pi}{4} Dh = 0.1885 \) mm³;

5. Initial side area: \( A_0 = \pi h \sqrt{\frac{D^2 + d^2}{2}} + \pi dD = 2.9635 \) mm².

In order to determine \( u_e \), one follows the reasoning described below. It is noted with \( \delta \) the thickness of the burnt powder layer, the same on the entire combustion surface of the element according to the geometric law hypothesis. Depending on the thickness of the burnt layer, the remaining volume of powder is given by the relation:

\[
V = \frac{\pi}{4} (D - 2\delta)(d - 2\delta)(h - 2\delta)
\]

which after processing becomes:

\[
V = 2\pi \left[ \delta^3 - \frac{D + d + h}{2} \delta^2 + \frac{Dd + dh + hD}{4} \delta \right] + V_c
\]

The fraction of burnt powder is defined:

\[
\psi = \frac{V - V_c}{V_c} = 1 - \frac{V}{V_c}
\]
The relation (24) can be put in the form of an algebraic equation of third degree, in which the relative thickness of the powder coated layer is unknown.

So:

\[ x = \frac{\bar{h}}{h} x^3 \left( \frac{D + d + h}{h} x + \frac{Dd + dh + hD}{h^2} \left( x^4 - \frac{\pi}{4} \frac{V_0}{h^3} \right) \right) = 0 \]  

(26)

At deflagration, \( x \) is between 0 and 1. Solving the dimensionless equation (26) is done by reducing to an equation of second degree of the form.

\[ \frac{D + d + h}{h} x^2 + \frac{Dd + dh + hD}{h^2} \left( x^4 - \frac{\pi}{4} \frac{V_0}{h^3} \right) = 0 \]  

(27)

Equation is put in the form of:

\[ \alpha x^2 - \beta x + \gamma = 0 \]  

(28)

in which: \( \alpha = \frac{D + d + h}{h} \), \( \beta = \frac{Dd + dh + hD}{h^2} \cdot \frac{\pi}{4} \), \( \gamma = x^4 - \frac{\pi}{4} \frac{V_0}{h^3} \).

The solution of the equation is in the form:

\[ x = \frac{\beta - \sqrt{\beta^2 - 4\alpha\gamma}}{2\alpha}, \]  

or after numerical replacements

\[ x = \frac{14.89 - \sqrt{221.7121 - 248.92\psi + 28x^2}}{14} \]  

(29)

The above equation is solved numerically, iteratively. In the first step, choose for \( x \) a value between 0 and 1 and enter \( (x_i) \) it into the equation. The new \( x \) \( (x_{i+1}) \) is thus determined. The calculation stop condition is \( x_{i+1} - x_i < 1e-6 \).

Depending on the thickness of the burnt layer, the area of the combustion surface is given by the relation:

\[ A_0 = \gamma_0 (\mu - \gamma_0) \sqrt{\frac{(d - 2\delta)^2 + (D - 2\delta)^2}{2} + \frac{\pi}{2} \frac{(d - 2\delta)(\mu - \gamma_0) (\mu - 2\delta)}{2}} \]  

(30)

The relation (27) expresses the area of the combustion surface according to the fraction of burnt powder, by the thickness of the burnt powder layer.

b. Equivalent powder

The equivalent powder element is considered to be spherical in shape, with combustion on the surface and has the dimensions:

1. Element radius: \( R_e = 5.3 \) mm;
2. The initial volume of the element \( V_{oe} = \frac{4}{3} \pi R_e^3 = 623.6145 \) mm³
3. Initial area \( A_{oe} = 4\pi R_e^2 = 352.9094 \) mm²

If \( r \) is the radius of the section at a given time, the fraction of burnt powder for the equivalent powder is written:

\[ \psi = 1 - \left( \frac{r}{R_e} \right)^3 \]  

(31)
Depending on the fraction of powder burned, the area of the combustion surface has the expression:

\[ A_2 = A_0 e^{(1 - \psi)^2} \]  \hspace{1cm} (32)

From the equivalence conditions, it follows that for the same fraction of burnt powder, \( \psi \), and the same pressure, the amount of gases generated must be the same. Note the combustion coefficient for the real powder with \( u_1 \) and with \( u_{1e} \) for the equivalent powder, then from the above condition it results:

\[ u_{1e} = \frac{A}{A_2} u_1 \]  \hspace{1cm} (33)

The calculation formula for the coefficient of combustion rate of the equivalent powder looks like this:

\[ u_{1e} = \frac{n_{rel} [2\pi (h - 2\theta)] \left( \frac{(d - 2\theta)^2 + (D - 2\theta)^2}{2} + \frac{\pi}{2} (d - 2\theta)(D - 2\theta) \right)}{A_{2e} (1 - \psi)^3} u_1 \]  \hspace{1cm} (34)

where: \( n_{rel} \) - number of real elements, \( \theta = \frac{h}{2} \) and \( x = \frac{14.89 - \sqrt{111.711 - 14.89^2}}{14.89} \).

In conclusion, the law of combustion of the equivalent powder is kept in the same form as the law of combustion of the real powder, with the difference that, the coefficient of burn rate, constrained by the conditions of equivalence, becomes a function of the fraction of burnt powder.

The limit values of the coefficient of burn rate of the equivalent powder are:
- for the beginning of burning \( x = 0 \) and \( \psi = 0 \)
- when it finished burning \( x = 1 \) and \( \psi = 1 \)

\[ u_{1e} = 2u_1 \]
\[ u_{e1} = 112.2u_1 \]

Equivalents equations obtained were implemented in FLUENT program by user defined functions written in C++ programming language.

3.3. Domain’s discretization

The FLUENT program numerically simulates the phenomena that occur in the fields occupied by the fluid, when they are subject to certain transformations. The basis of the methods used in the FLUENT program is represented by the finite volume or control volume calculation techniques. The technique of finite volumes approach involves dividing the domain occupied by the fluid into subdomains of simple form, figures or elementary geometric bodies (for 2D problems, triangles, quadrilaterals and for 3D problems, tetrahedra, prisms, hexahedra).[6]

The system of equations implemented within the program, which includes continuous field variables such as velocities, pressure, temperature, density is subject to discretization transformations. In this process the continuous fields are replaced by discrete fields of values defined in the centers of the control volumes. The FLUENT program operates with the discrete set of these variables. The accuracy of the solutions is conditioned by the domain discretization. A refined domain leads to higher computing accuracy, instead it involves a larger computing effort.[7]

For the numerical simulations, a model of the 10 \( \text{cm}^3 \) closed vessel was developed in the two-dimensional case, specifying the constructive elements as can be seen in figure 5.

The analysed model was discretized using triangular elements for both domains, also using a boundary layer as can be seen in figure 4 and figure 5.
Figure 5. Equivalent physical model of the 10 $\text{cm}^3$ closed vessel used in numerical modelling – detail: 1 - inside the closed vessel; 2-wall; 3 - boundary layer; 4 - equivalent powder element; 5 - primer of black powder.

In the analysed case, due to the variable internal configuration, a dynamic mesh was used that allows the domain to be transformed according to how the powder’s elements deflagration evolves, so that at any moment of the phenomenon’s analysis, the field occupied by the combustion products is occupied of finite volumes with controlled dimensions. To discretize the field of combustion products from the analysed system, one can use structured, unstructured or mixed finite volume networks. In the numerical analysis applied in the paper we used a triangular network with boundary layer (figure 4 and figure 5) whose characteristics at the initial time point ($t = 0$) are presented in table 1:

| $t = 0$ s | Level | Cells | Faces | Nodes | Partitions |
|----------|-------|-------|-------|-------|------------|
| 0        | 30226 | 47116 |       | 16891 | 1          |

Table 1. Data regarding domain’s discretization at the beginning of the simulation.

The triangular elements used present the advantage of better control of dynamic discretization. During the simulation due to the permanent modification of the working area there was a variation of the number of elements as follows in table 2:
Table 2. Data regarding domain’s discretization at the end of the simulation.

| t = 2.6 ms | Level | Cells  | Faces  | Nodes  | Partitions |
|-----------|-------|--------|--------|--------|------------|
| 0         | 51432 | 67216  | 24792  | 1      |            |

2 cell zones, 17 face zones

4. Results
In order to determine the burning law, we fired in the closed vessel in the same conditions. The results obtained are presented in the figure 6.

The simulation was conducted in several cases, u₁ and v being modified, iteratively, in order to obtain a good accord with experimental values. After the numerical simulation process, we obtained the variations of pressure function of time, as you can see in the figure 7.

Figure 6. The variation of pressure function of time obtained from experimental.

Figure 7. The variation of pressure function of time obtained from numerical simulation.
To determine which theoretical curve offers a better approximation of the experimental one we used least squares method implemented in Matlab software. Burning law equation in the simulated case has the following form:

$$u = 0.22 \cdot p$$  \hspace{1cm} (35)

We obtained also the variation of temperature and burning surface of powder function of time. The results are presented in the figure 8 and figure 9.

Figure 8. The variation of temperature function of time obtained from numerical simulation.

Figure 9. The variation of burning surface function of time obtained from numerical simulation.

5. Conclusions
In this paper, it was presented a method to determine the burning rate law for small caliber ammunition powder using numerical simulations. Due to conditions from the physical domain of closed vessel and in order to obtain a fast solution, we elaborate a simulated axis-symmetrical model.
Starting from physical dimensions of the real powder, which can be elliptical, cord, ball, flake, single perf etc. we generate an equivalent spherical element powder for which we calculate the equivalent conditions from real case. Equivalents equations obtained were implemented in FLUENT program by user-defined functions written in C++ programming language.

The theoretical results obtained using numerical simulations were compared to the experimental data, being in good accord with the experimental results. This method is a very useful tools for design the propulsive charge giving also the variation of temperature, burning surface, burning fraction etc. as a function of time and combustion thickness.

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