

# Simulation of energetic composite materials combustion

Yu. Dimitrienko<sup>1\*</sup>, A. Zakharov<sup>1</sup>, and M. Koryakov<sup>1</sup>

<sup>1</sup>Bauman Moscow State Technical University 5, 2-ya Baumanskaya str., 105005 Moscow, Russian Federation

**Abstract.** A numerical approach to simulate the evolution of the combustion surface of an energetic composite materials is described. Cubic spline interpolation is used to describe the dynamically changing shape of the combustion surface. The statement of the interpolation problem for the parametric description of the geometry and the problem of choosing the method for parameterizing the control points are given. The direct step-by-step method is used to calculate the combustion front. The normal velocity of the combustion surface is variable and is determined from the solution of an additional gas dynamics problem. The basic formulae for calculating the combustion rate of a solid propellant that consists of a particle-reinforced energetic composition are given. Examples of combustion simulation of a laboratory-scale structure for three values of the initial geometry parameters are presented. **Key words:** energetic composite materials, geometric modeling, combustion.

## 1 Introduction

Energetic composite materials are widely used in aerospace industry. One of the most important problems encountered in the design of energetic compositions is the modeling of the complex processes that occur during the grain combustion, when various factors that influence the final efficiency of the designed propellant grains must be taken into account.

These factors include the following: (1) The complexity and variability of the geometric shape of the combustion surface, where even the connectivity of the surface changes; (2) The dependence of the combustion rate on a large number of different parameters: pressure of the gaseous products in the internal cavities, mechanical and thermophysical properties of the energetic compositions, as well as on the features associated with the grain manufacturing technology and the initial state of the grain components.

The above factors mean that the combustion rate depends not only on time but also on the three-dimensional spatial coordinates. In some cases, propellant parts may not be connected to each other, resulting in multiply connected combustion surfaces. Furthermore, the surface connectivity and regularity can change during the grain combustion.

Different methods are currently used to simulate grain evolution. The level-set method [1-7] is based on the numerical solution of the differential equation of motion of a phase

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\* Corresponding author: [dimit.bmstu@gmail.com](mailto:dimit.bmstu@gmail.com)

interface in the actual configuration [8-9]. The level-set method is good at computing and analyzing the motion of the interface in two or three dimensions. However, the use of an artificial viscosity in solving the nonlinear equation of motion of the interface leads to problems in the approximation and stability of the numerical method.

The MDF method [10–11] is based on calculating the distances between two grids: a volumetric grid in the grain domain and the gas flow within it, and a triangulation grid over the area covered by the combustion surface. The main disadvantage of this method is the computational complexity.

A spectrally accurate description of the combustion surface was discussed in [12]. Algorithms for the removal of appearing loops in two or three dimensions are considered. For this purpose, self-intersections of the grain contour are detected and it is determined which markers are inside the multivalued zone and which ones are on the exterior of the contour.

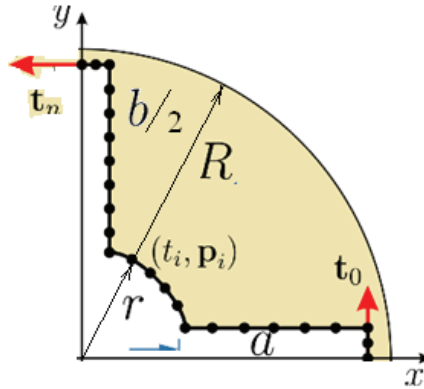
The three methods namely the front-tracking, emanating-ray, and least-distance methods, were proposed in [13] to track the regressing surface. The methods of emanating rays and the front-tracking require a priori assumption about the object's topology and are therefore not universal. The least distance method requires a background grid placed over the volume of space occupied by the energetic composition.

Numerical methods for coupled problems of fluid dynamics and elasticity were examined in [14-16]. These methods make it possible to determine the parameters of the gas flow acting on the structure and the response of the material to these forces. These parameters are used in calculating the combustion rate of energetic composition.

In this study we develop a method and perform a simulation of the evolution of the combustion surface. We use the equation of the motion of the phase interface written in a locally linearized form at each time step. This approach makes it possible to simplify the solution of the original equation of the motion of the combustion surface and to overcome the problems encountered in the numerical solution. One of the problems encountered in this approach is the need to remove loops formed during the concave grain combustion. The paper considers one of the effective algorithms to solving this problem. We apply cubic interpolating splines written in parametric form to describe the shape of the curved combustion surface and its motion. The use of these splines makes it possible to describe a wide variety of energetic composition geometries.

## **2 Representation of the initial geometry of the combustion surface**

A typical energetic composition is a cylindrical body with several slots [17-19] (Fig. 1). During the combustion process, the inner surface of the energetic composition moves with a variable normal velocity. We will use the parametric form of the equations describing the propellant grain boundaries. We will interpolate the boundaries with cubic splines.



**Fig. 1.** Cross section of a cylindrical propellant grain made of energetic composition.

Consider the problem of finding the functions of a cubic spline  $\mathbf{r}(u) = [x(u), y(u)]$  given by the set of control points  $(u_i, \mathbf{p}_i)$ ,  $i = 0, \dots, n$ . Specify a cubic spline function for each coordinate (x or y), denoting it as  $S(u)$  in the form of the following polynomial expression

$$S(u) \equiv S_i(u) = a_i(u - u_i)^3 + b_i(u - u_i)^2 + c_i(u - u_i) + d_i \quad (1)$$

on every interval  $u \in [u_i, u_{i+1}]$ ,  $i = 0, \dots, n-1$ .

Consecutive polynomials are smoothly adjusted

$$S_{i-1}^{(k)}(u_i - 0) = S_i^{(k)}(u_i + 0), \quad i = 1, \dots, n-1, \quad k = 0, 1, 2. \quad (2)$$

The interpolation conditions are satisfied

$$S(u_i) = p_i, \quad i = 0, \dots, n. \quad (3)$$

The remaining two free parameters are usually determined from the restrictions on the value of the spline and its derivatives at the endpoints of the interval  $[u_0, u_n]$  (or near its ends) [20]. Since the cylindrical grain with slots forming a cross shape is axially symmetric, we calculate only one quarter of the combustion surface (Fig. 1).

Then, the tangent vectors can be assigned at the ends of the cubic spline curve:

$$S'(u_0) = p'_0, \quad S'(u_n) = p'_n. \quad (4)$$

Let the tangent vectors are

$$\mathbf{p}'_i = \alpha_i \mathbf{t}_i, \quad \|\mathbf{t}_i\| = 1, \quad i = 0, n. \quad (5)$$

Due to the symmetry constraints, their directions  $\mathbf{t}_i$  are obviously equal to those in Fig. 1. The magnitudes of the tangent vectors  $\alpha_i$ , should be roughly the average speed over the end segments

$$\alpha_0 = \frac{\|\mathbf{p}_1 - \mathbf{p}_0\|}{u_1 - u_0}, \quad \alpha_n = \frac{\|\mathbf{p}_n - \mathbf{p}_{n-1}\|}{u_n - u_{n-1}}. \quad (6)$$

The solution to this interpolation problem is given for example in [20-22].

Since the geometry contains slightly rounded corners (Fig. 1), the centripetal method was chosen for parameterizing the control points

$$u_0 = 0, \quad u_n = 1, \quad u_i = u_{i-1} + \frac{\sqrt{\|\mathbf{p}_i - \mathbf{p}_{i-1}\|}}{d}, \quad i = 1, \dots, n-1; \quad (7)$$

where

$$d = \sum_{i=1}^n \sqrt{\|\mathbf{p}_i - \mathbf{p}_{i-1}\|}. \quad (8)$$

Lee et al. have shown that even with a small number of control points it gives a better approximation to this geometry [22].

### 3 Calculation of combustion rate

The combustion of energetic compositions is associated with the thermomechanical decomposition of fuel binder under the action of two factors. The first one is the internal pressure of gaseous products of thermal decomposition of the fuel and oxidizer. The second factor is the impact of an external gas flow which moves along the combustion surface and leads to shearing of solid particles [24].

The speed of displacement of the combustion surface along the internal normal to it is called the linear combustion rate and is denoted by  $D$ . The proposed model for its calculation is able to take into account both external pressure and flow velocity.

We can represent the linear combustion rate  $D$  of propellant as a sum of rates  $D_e$  and  $D_i$  of these two processes [9, 24]

$$D = D_e + D_i \quad (9)$$

where  $D_e$  – external thermomechanical erosion rate,  $D_i$  – internal thermomechanical erosion rates caused by the destruction of fuel binder under the pressure of gaseous products of solid propellant thermal decomposition [9, 24]

$$D_e(\theta_s, p_\Sigma) = \frac{1}{\rho_s} \left( \frac{J_s^0 \lambda_s}{c_s} \right)^{1/2} \left( \frac{6p_\Sigma}{\sigma_T} \right)^{\alpha_1} \left( \frac{R\theta_s}{E_s} \right)^{1/2} \exp\left( -\frac{E_s}{2R\theta_s} \right), \quad (10)$$

$$D_i(\theta_s) = \left( \frac{J_s^0 \lambda_s}{c_s \rho_s} \right)^\omega \left( \frac{6 \rho_s l_0}{K \sigma_T} \right)^{2\omega-1} \left( \frac{R \theta_s}{E_s} \right)^{1/2} \exp\left( -\frac{E_s \omega}{R \theta_s} \right), \quad (11)$$

where  $\rho_s$ ,  $\lambda_s$ ,  $c_s$  are effective density, heat conductivity and heat capacity of the composite propellant;  $J_s^0$  is the preexponential multiplier and  $E_s$  is the activation energy of thermodecomposition process of the composite matrix;  $\sigma_T$  is the strength of the composite at temperature  $\theta_s$ ,  $K$  is the gas permeability coefficient of the composite at temperature  $\theta_s$ ;  $l_0$  is the characteristic diameter of pores or gas bubbles formed during the thermal decomposition of the fuel and oxidizer,  $R$  is the gas constant,  $p_S = p + r_g \left| \mathbf{v}_g \right|^2$  is the total pressure of flow, consisting of a static pressure  $p$  and dynamic pressure component,  $r_g$  is the density of the gas phase,  $\mathbf{v}_g$  is the velocity of gas phase flow. Dynamic pressure is due to the motion of the flow in the internal cavities of the propellant combustion. The method for calculating flow parameters is described in [14-16].

The radius vector of points of the combustion surface is denoted as  $\mathbf{r}(u,v,t)$ , where  $t$  is the time and  $(u,v)$  are the parametric coordinates on the surface. To calculate the combustion front, we will use an ordinary differential equation in the form

$$\frac{\partial \mathbf{r}}{\partial t} = D \mathbf{n} = D \frac{\mathbf{r}_u \times \mathbf{r}_v}{\|\mathbf{r}_u \times \mathbf{r}_v\|}, \quad (12)$$

where  $\mathbf{r}_u = \frac{\partial \mathbf{r}}{\partial u}$  and  $\mathbf{r}_v = \frac{\partial \mathbf{r}}{\partial v}$  are the tangent vectors of the combustion surface.

## 4 Algorithm for grain combustion simulation

The algorithm for grain combustion simulation consists of the following steps:

1. Generate the Cartesian and parametric coordinates  $(u_i, \mathbf{p}_i)$ ,  $i = 0, \dots, n$  of the control points. Construct the spline  $S^0$  of the initial combustion surface.
2. Draw the spline geometry, calculate the combustion area from unburned portions of the spline surface.  
Go to the next time step. Calculate the new positions of the control points according to their unit normal vector and linear combustion rate.
3. Check the condition that the new radius  $r$  of a control point is not larger than the radius  $R$  of the interior chamber cylindrical wall. Control points that do not satisfy this condition are marked as burned. We assume that  $r = R$  for burned points. The portions between the burned points are also considered as burned.
4. Remove forming loops (see below).
5. Recalculate the parametric coordinates of the remaining control points.
6. Construct the spline  $S^1$  of the modified combustion surface.

7. Restore the original number of control points. To do this, we generate the Cartesian and parametric coordinates  $(u_i, \mathbf{p}_i)$ ,  $i = 0, \dots, n$  of the new control points according to the obtained spline  $S^1$ .

8. Construct the new spline  $S^2$  of the modified combustion surface.

9. Return to step 2 if the combustion area is not zero.

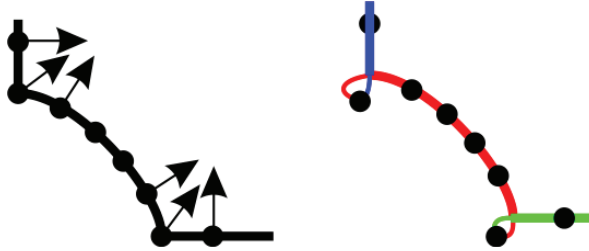


Fig. 2. The forming of loops.

Since the geometry of a combustion surface is concave, moving portions near the inner corners will form loops (see Fig. 2) that must be removed. The following algorithm is used for this purpose.

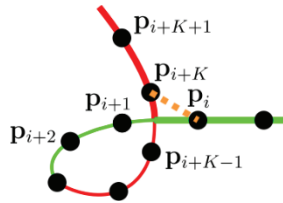


Fig. 3. Loop finding.

For each control point  $\mathbf{p}_i$  calculate the distance to all following points

$$s_k = \|\mathbf{p}_{i+k} - \mathbf{p}_i\|, \quad k \geq 1. \quad (13)$$

If the condition

$$s_k \leq s_1 \text{ for } k > 1 \quad (14)$$

is true, then save the value of  $k$ . Find the maximum value  $K$  of all  $k$  that satisfy (14). Set the point  $\mathbf{p}_K$  as the end point of the loop (Fig. 3). Exclude the points  $\mathbf{p}_{i+1}, \dots, \mathbf{p}_{i+K-1}$  from the set of spline control points to remove the loop.

## 5 Results and discussion

We have developed software that allows researchers to enter the geometric and physicochemical parameters of a grain, display the animation of the change in geometric shape during grain combustion, calculate the combustion area and save it in a text file at any time. We have used the JavaScript language and Three.js graphics library [25-27].

We have examined three case studies of the slot geometries of the grain, which are shown in table 1 and figure 1. All parameters are dimensionless. In all cases, the ignition of the grain was assumed to occur immediately over the entire inner surface of a grain.

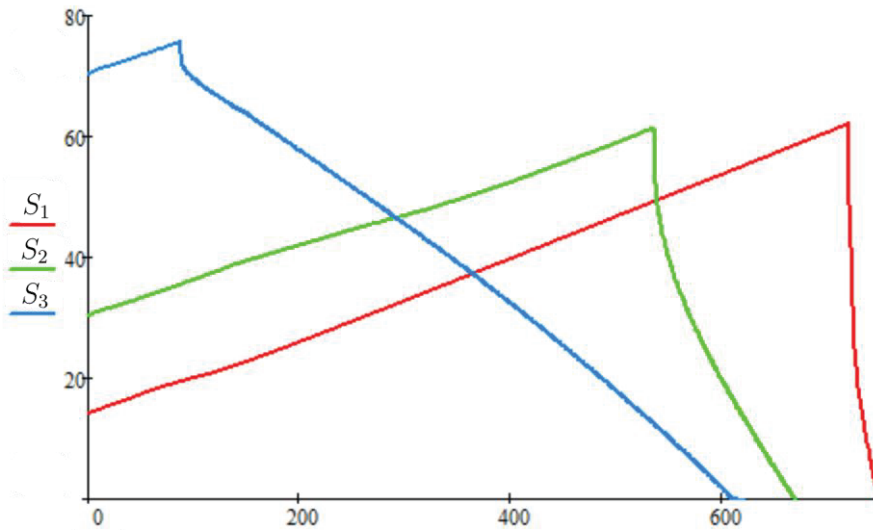
**Table 1.** Values of the geometric parameters of the grain used for the three case studies.

Case study number	a	b	r	R
1	1	1	1	10
2	3	0.5	1	10
3	8	0.5	1	10

The slot length is small and equal to the thickness. During the grain combustion, the combustion area increases monotonically starting from a rather small value, increasing to a maximum value at the outer boundary of the grain and corresponding to the moment of almost complete grain burnout. The combustion is progressive and the combustion time is the maximum time among all the considered case studies.

In the third case study, the slot length is sufficiently large. The combustion surface quickly reaches the outer boundary of the grain. Then it is divided into four separate parts and becomes multiply connected. The combustion area begins to decrease monotonically, so that the combustion is regressive (Fig. 4). The combustion time of the grain is the shortest.

The slot length used for the second case study is between that of the first and third case studies. The initial combustion area is almost twice as large as the one in the first case study. Just as in the first case study, the combustion area increases monotonically, the combustion is progressive, but the combustion time of the grain is 11 percent less than in the first case study.



**Fig. 4.** Combustion area with respect to the time for the all three case studies.

## 6 Conclusion

1. A geometric model has been developed to describe the change in curved boundaries of the combustion of energetic compositions. The method is based on a spline interpolation technique and a direct method for numerically solving the equation of the motion of the phase interface.

2. The method used is much simpler and more efficient than ones using the original nonlinear equation of motion of the interface. This allows the animation of the change in the combustion front to be displayed in real time. The use of splines makes it possible to describe a sufficiently large class of solid propellant grain geometries, including those that have corner regions of large curvature.
3. A program has been developed to calculate and visualize the evolution of a grain geometry. The program runs on a regular browser and has a user interface for entering the geometric and physicochemical parameters of the grain.
4. Numerical simulations of the dynamically changing shape of the combustion surface have been carried out for three values of the initial geometry parameters of the laboratory-scale energetic compositions. Dependencies of the combustion area on the time have been obtained, and a type of combustion has been determined for each case study.

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