Mathematical model and software for investigation of internal ballistic processes in high-speed projectile installations

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Mathematical model and software for investigation of internal ballistic processes in high-speed projectile installations

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Abstract. This paper describes a software package that allows to explore the interior ballistics processes occurring in a shot scheme with bulk charges using propellant pasty substances at various loading schemes, etc. As a mathematical model, a model of a polydisperse mixture of non-deformable particles and a carrier gas phase is used in the quasi-one-dimensional approximation. Writing the equations of the mathematical model allows to use it to describe a broad class of interior ballistics processes. Features of the using approach are illustrated by calculating the ignition period for the charge of tubular propellant.

1. Introduction
Applying of new high-energy propellants, complex designs of missile assemblies, ballistic installations on new physical principles requires constant improvement of mathematical models describing internal ballistic processes [1-3]. Mathematical models that adequately reflect the processes that occur during the shot process are most in demand in the formation of shot parameters predictive estimates in the extreme ranges of experiments.

In the presented mathematical problem formulation, a model of a polydisperse blend of non-deformable particles and a carrier gas phase moving along a channel of a spatial coordinate alternating cross section in a quasi-one-dimensional approximation is used [1]. During writing of the equations, it is assumed that the viscosity and heat conductivity of the gas are manifested only in interaction with the particles. It is also assumed that layer-by-layer burning of the powder propellant charge elements occurs at a velocity depended only on the temperature of the powder gases.

2. The basic system of gasdynamic equations
The basic system of equations that determines internal ballistic processes is written in a form that allows them to be used for a wide class of problems describing internal ballistic processes.

2.1. Equations expressing the laws of conservation of mass, momentum, and energy
It's as if there are particles of \( J \) varieties that differ in size and other characteristics. The gas is a homogeneous blend of \( J \) non-viscous non-heat-conducting gases with known equations of state, each of which is formed by the combustion of a particle of the corresponding kind.

Let us introduce the following notation:
- \( t \) - time;
- \( x \) - spatial coordinate measured along the axis of the axisymmetric barrel bore in the direction of throwing;
s(x)- channel cross-sectional area;
ρ_j - average density of the gases formed during the combustion of the particles j-th kind;
ρ^0_j - истинная плотность j-го газа;
ρ = \sum_{j=1}^{J} ρ_j - average density of a homogeneous blend of gases;
ρ^0 - true gas blend density;
c_j = ρ_j / ρ - a mass fraction of the j-th gas in the gas blend \left(\sum_{j=1}^{J} c_j = 1\right);
α_j - volume fraction of j-th gas in the gas blend \left(\sum_{j=1}^{J} α_j = α\right);
δ_j - true density of the j-th kind of particles;
β_j - volume fraction of the j-th kind of particles in the gas-powder blend \left(\sum_{j=1}^{J} β_j = β = 1 - α\right);
u_j - velocity of the j-th kind particles;
p, T, u - respectively, the pressure, temperature and velocity of the gas blend.

The motion of the polydisperse blend along the channel of the alternating cross section is described by the laws of conservation of mass, momentum, and energy, the form of which is given below.

For each component of the homogeneous gas blend
\[ \frac{∂}{∂t} (ρ_j s) + \frac{∂}{∂x} (ρ_j u s) = m_{ij} s \quad (j = 1, ..., J), \] (1)
summing which, we have the law of conservation of the gas phase mass
\[ \frac{∂}{∂t} (ρ s) + \frac{∂}{∂x} (ρ u s) = \sum_{j=1}^{J} m_{ij} s \] (2)

For each kind of particles, we have
\[ \frac{∂}{∂t} (β_j δ_j s) + \frac{∂}{∂x} (β_j δ_j u_j s) = m_{pj} s \quad (j = 1, ..., J) \] (3)

There is \( m_{ij} (m_{pj}) \) - mass inflow of the j-th gas (particles) per unit time, per unit volume of the blend.

An equation
\[ \frac{∂}{∂t} (ρ u s) + \frac{∂}{∂x} (ρ u^2 s) = -α s \frac{∂p}{∂x} + 2πRσ_\| - s \sum_{j=1}^{J} (f_j - m_{ij} u_{ij}) \] (4)
is the law of conservation of momentum for the gas phase, and
\[ \frac{∂}{∂t} (β_j δ_j u_j s) + \frac{∂}{∂x} (β_j δ_j u^2_j s) = -sβ_j \frac{∂p}{∂x} + s (f_j + m_{pj} u_{pj}) \] (5)
for the j-th fraction of particles.

Here the following notation is made: \( f_j \) - the force projection on the x-axis per unit blend volume with which the gas acts on particles of the first kind due to the difference in the phase velocities; \( u_{ij} (u_{pj}) \) - velocity of the gas (particles) entering in the polydisperse mixture; \( σ_\| \) - frictional stress in the gas at the channel surface.

For the gas phase, the energy conservation law in the form for the total energy has the form
\[
\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x} (\rho u E) = -\frac{\partial}{\partial x} (\rho u s) - \sum_{j=1}^{J} \frac{\partial}{\partial x} (p \beta_j u_j s) + s \sum_{j=1}^{J} u_j \left( \beta_j \frac{\partial p}{\partial x} - f_j \right) + s \sum_{j=1}^{J} m_{jg} \left[ Q_{gj} + \frac{u_{gj}^2}{2} \right] - s Q_j - sq
\]

(6)

Here \( E = e + \frac{u^2}{2} \) is total energy of gas blend;

\( e = \sum_{j=1}^{J} c_{e,j} e_{g,j} \) - internal energy of gas blend;

\( Q_{gj} \) - a specific internal energy of the gaseous combustion products entering the blend;

\( Q \) - an intensity of heat losses due to heat exchange with the walls of the barrel channel per unit volume of the blend;

\( q = \sum_{j=1}^{J} q_j, q_j \) - intensity of energy inflow to particles of the n-th grade per unit volume of the blend due to heat exchange with gas.

Similarly, for the j-th particles fraction

\[
\frac{\partial}{\partial t} (\beta_j \delta_j E_s) + \frac{\partial}{\partial x} (\beta_j \delta_j u_j E_s) = -u_j \left( \beta_j \frac{\partial p}{\partial x} - f_j \right) + sm_{pj} \left[ Q_{pj} + \frac{u_{pj}^2}{2} \right] + sq_j
\]

(7)

where is \( E_j = e_j + \frac{u_{j}^2}{2} \),

\( e_j \) - the specific internal energy of the particles (the known function of temperature);

\( Q_{pj} \) - the specific internal energy of the particles entering into the blend.

As can be seen from the structure of the equations, for the zero value \( m_{gj} \), or \( m_{pj} \), the corresponding values \( u_{gj} \), \( u_{pj} \) and \( Q_{gj} \), \( Q_{pj} \), \( Q_j \) can have any value except \( \infty \), since they enter the equations as a product with \( m_{gj} \), \( m_{pj} \).

Equations (1) - (7) for given values \( m_{gj} \), \( m_{pj} \), \( u_{gj} \), \( u_{pj} \), \( Q_{gj} \), \( Q_{pj} \), \( f_j \), \( q_j \), which determine the interphase interaction of gas-condensed particles; \( \sigma_w^a \), \( \sigma_q \) - specifying friction and heat exchange on the surface of the barrel; Equations of state of the gas blend \( e_j(T) \) and represents a closed system for determining the average densities of the gas components \( \rho_j \), the velocity \( u_j \), the volume content \( \beta_j \) and temperature of the particles \( T_j \), the pressure \( p \) and the velocity \( u \) of the gas blend. The arbitrary choice of the dependencies that determine the interfacial interaction, friction and heat transfer to the barrel, the state equation of the gas components and the solid phase makes it possible to use system (1) - (7) for modeling a wide class of internal ballistic phenomena. A number of types of particles can be distinguished a priori, for which either these dependences are trivial, or some of the equations (1) - (7) do not make sense.

3. Classification of particles by types

3.1. Burning particle

Particles of this type are used to simulate the burning elements of a propellant charge, the corresponding quantities \( m_{gj} \), \( \rho_j \), \( \rho_j^0 \) are nonzero. For calculating combustion, the ratios generally accepted in internal ballistics are used [4]:

\[
m_{gj} = -\frac{\beta_j \delta_j}{1 - \psi_j W_{gj}} \frac{s_{gj}}{\sigma_j(\psi_j)} U_j(p),
\]

(8)

where \( \psi \) is a degree of transformation;
s_0 – initial particle surface;
W_0 – initial volume of a particle;
\( \sigma(\psi) \) – ratio of the current burning surface to the initial;
U(p) – law of layer-by-layer combustion.

Calculation of the energy equation (7) for a particle is not made \( q_j = 0 \).

3.2. Non-burning particle

For non-burning, the intensity of the volumetric mass input of the gas \( m_{\text{gj}} = 0 \), the corresponding values of the average \( \rho_j \) and true \( \rho_j^0 \) density of the gas formed during its burning are also zero, equation (1) has no meaning. This type of particle is used to simulate soot in combustion products, condensed ablation products, etc. In the presence of particles of this type, it is necessary to calculate the energy equation (7) for a particle, and to take into account the nonzero value \( q_j \) in the energy equation (6) for a gas.

3.3. Particle absent

This is the case of a fictitious particle that is introduced in order to uniformly calculate the gas originally located in the channel, for example, the products of the igniter's combustion in the event that its formation is not calculated. Equations (3), (5), (7) are not calculated, \( m_{\text{gj}} = 0 \).

The writing of equations in the form (1) - (7) allows one to have particles of any types in one computational domain. In this case, for example, a type 1 particle can form gaseous products and condensed components as a result of combustion, each of which in turn can be of type 2 (soot) or type 1 (TC dispersing products). Therefore, from the point of view of logical organization and computer realization it is advisable to introduce the term "particle sets" (PS), which means a certain closed set of particles. By closedness we mean that particles from a particular PS are, firstly, intended to describe a single element of a mathematical model, and second, they occupy the same continuous sequence of indices in an array of particles, and, thirdly, for them in the calculation process the quantities \( m_{p_j}, m_{g_j}, u_{p_j}, u_{g_j} \) are mutually consistent.

The simplest example of the PS is the model of the powder charge element, in the combustion of which only the gaseous component is formed. In this case, only one index \( j = k \) corresponds to this "particles sets", the velocities of the burning particle and its combustion products equal \( (u_{p_k} = 0, \ u_{g_k} = u_k) \), and the intensities of the bulk gas arrival and the decrease in the mass of particles are equal in magnitude \( (m_{g_k} = -m_{p_k}) \) and are determined from (8).

In a more complicated case of combustion of a powder charge element with the formation of combustion products and one condensed component with a mass fraction, two components of a polydisperse blend (for example, one with an index \( j = k \), the other with \( j = l \)) are required to describe this PS as the first for describing the element of the powder charge itself, for the resultant condensed particle. Here the following relations are satisfied
\[
\begin{align*}
m_{g_k} &= -m_{p_k}, \quad u_{p_k} = 0, \quad u_{g_k} = u_k, \\
m_{p_l} &= -m_{g_l} c, \quad u_{p_l} = u_k, \quad u_{g_l} = 0, \quad m_{g_l} = 0,
\end{align*}
\]
where \( m_{p_k} \) determined by (8).

Similarly, other "particle sets" are constructed, for example, to describe particles that are carried by a gas stream from a melting surface of a barrel or from dispersed products of TC.

The dependences that determine the strength and thermal interfacial interaction of gas and spherical particles are given in [1]. Introducing the particle bareness as a ratio of its surface to volume and writing the expression for \( f_j \) in a form generally accepted for the problem of external flow past a spherical particle, we have
\[ f_j = \rho^0 \beta_j s_p C_d \frac{|u - u_j|}{8} (u - u_j) \]  \hspace{1cm} (9)

For grains of powders, taking into account the disorder in their packing and neglecting the influence of the velocity field of the combustion products flowing from the particle, a dependence of the form (9) is also used for the interphase interaction force.

For the resistance force of tubular and rod powders, a dependence of the form (9) is used, in which the resistance coefficient corresponds to the experimental dependences for packets of pipes that are streamlined in the longitudinal direction [5].

For the dependence of the particle surface on the transformation degree \( \frac{s_0}{W_0} \sigma(\psi) \), a number of constraints are used that express the various geometric and physical laws of gas formation. A power pressure dependence is used for the linear combustion rate.

Friction and heat exchange with the barrel during gas motion are determined by semiempirical criterial dependencies obtained for the stationary flow regime. In this case, the temperature distribution in the thin heated layer of the barrel material is determined from the solution of the one-dimensional heat conduction problem in the cross sections of the barrel.

The system of equations (1) - (7) is solved numerically with the corresponding initial and boundary conditions.

Initial conditions:
\[
\begin{align*}
 p(x,0) &= p_0; & u(x,0) &= 0; & T(x,0) &= T_0; \\
 \rho_j(x,0) &= \rho_0; & (j = 0 \div J); \\
 \beta_j(x,0) &= \beta_0(x); & u_j(x,0) &= 0; & (j = 1 \div J),
\end{align*}
\]

where \( \rho_0, p_0, T_0 \) are parameters characterizing the initial state of the gas phase;

\( \beta_0(x) \) sets the initial spatial distribution of the j-th fraction due to initial placement propellant elements.

In the simulation of internal ballistic processes, calculations performed on the developed mathematical model are carried out in the region bounded to the left by the charging chamber bottom cross section, and to the right by the projectile left end cross-section for the classical charging scheme or the combustion front for the charging scheme with the traveling charge.

In the section of the loading chamber bottom, the non-flow conditions are set.

When specifying the boundary conditions for the classical loading scheme, the projectile also specifies non-flow conditions. For the charging scheme with the traveling charge, the conditions given in [1] are used.

The above mathematical formulation is solved numerically by modifying the Godunov method, allowed to increase the approximation order on the spatial coordinate to the second order [6] and the time second order [7], and implemented as a software package (PC). When it was created, modern technologies for developing software systems were used.

Progress in the field of programming languages (PL) and development tools has made it possible to significantly simplify the development process and give the software new properties. At present, a more modern object-oriented approach has come to replace the technology of structural programming implemented in the PL, such as Algol, Fortran, Pascal, which facilitates programming, debugging and testing, support and further modification. The most convenient for implementing software systems developed within this approach are the PL, which support the style of object-oriented programming. Among them, the most common is C ++, which has a number of advantages over other object-oriented languages. Firstly, it is a compiled PL that combines the features of a high-level PL with the ability to perform low-level data operations and allows you to create high-speed programs. Secondly, compilers with C ++ exist on almost all computing platforms.
The essence of the object-oriented approach in the development of software systems for modeling the concepts and phenomena of the surrounding world consists in constructing their abstract models based on the selection of properties essential for the development purpose. If the simulated phenomenon is complex, then the models of its components are built, and the developed software system is considered as a composition of abstract models of its components. In C++, the representation of an abstract model is a class, in fact it is a data type defined by a developer programmer to model a concept or phenomenon. The class contains data components and methods (functions) for working with data. An instance (an object in C++ terms) of a class can be created in the main memory of a computer. Classes can be among themselves in relation to generalization or inheritance, allowing to identify analogies between them and to build a multi-level classification in relation to "general - private" (class hierarchy). A class that is closer to the top of the hierarchy (base class) is the bearer of more general properties with respect to classes located further from the top of the hierarchy (derived class). This is expressed in the fact that an object of a derived type always contains a subobject of the base type in its composition, while the same properties (data-components) for objects of the base and derived types have the same offsets relative to the initial address of the object. This allows you to view derived type objects from general positions (as objects of the base type), while using the technology of virtual functions when working with objects allows you not to lose the individuality inherent in objects of the derived type. It is possible to associate types belonging to different hierarchies for collaboration, using pointers (that is, addresses) to these or basic types. The set of hierarchies of classes constructed in this way, characterizing various aspects of the modeled domain, determines the functional content of the software package (PS). Obviously, using this development technology makes it easy to modify the composition of software by adding or excluding classes from the hierarchy. Very important is the ability to construct and destroy objects of an abstract type dynamically, while the program complex is running, which allows you to create a set of objects for solving a particular problem, guided by the specification of a set of input data.

With respect to mathematical modeling of processes in gas-dynamic propellant devices, the first level of abstraction is determined by the choice of physico-mathematical models describing the phenomenon and numerical methods for their solution. The described technology of software systems development is applied at the stage of software implementation for computer modeling of the subject domain under consideration. To do this, you need to define, for example, the following hierarchy of concepts, taking into account the multivariate types involved in the hierarchy:

- the calculation area together with the system of calculated equations and the calculation method (abbreviated as "calculation area");
- boundary condition (abbreviated as "boundary");
- installation geometry;
- resistance law;
- laminar burning rate;
- relative particle area;
- particle;
- multitude of particles;
- computing task;
- result output.

When implementing the software, the Qt library [8] was used, this library allows to create mobile software for various operating systems based on a single code written in PL C++.

The software package is an application that runs on Windows. The main window of the PC can be in one of two modes: in the activated mode of calculation (in this case, the graphic output, which illustrates the calculation process, outputs to the client part of the main window) and in the inactive mode. In the first case, within the computational process, a workflow is created that performs calculations, the primary stream serves the output of graphic information and the operation of the data preparation subsystem (DPS). Thus, the software package is a two-stream application for Windows.
During the calculation, the execution of both threads is synchronized using standard Qt (mutexes and waiting conditions). The toolbar view in the calculation execution mode is complemented by the workflow management tools and visualization of the calculation results. In the inactive mode, the following options are available on the toolbar: calling the settings window and the DPS window.

The subsystem of data preparation allows to work on creation, editing and saving of a set of computational configurations, which represent a data set characterizing the realized mathematical and information model. The sets of data included in the design configuration must have the property of mutual consistency. This means that, being formally independent, they enter into a single design configuration, where different parts of the mathematical and information model implemented in the PC cannot be set independently of each other. An example is the placement of elements of a propellant charge whose left boundary cannot be less than the coordinate of the powder chamber bottom specified by the type "Internal geometry of the barrel", and the right boundary cannot be greater than the right boundary of the design area, which is determined by the types "Projectile with friction and backpressure" and "Travelling charge".

The difference between the developed mathematical model and those given in [2, 3] is that the description of internal ballistic processes is based on a single system of equations written for an arbitrary number of particles, each of which is included in the MF. The software implementation allows specifying, changing and adding to the program complex new possibilities practically without processing the existing program code. This can be illustrated with the example of calculating the pipe powder charge ignition period in the formulation [3].

The ignition period calculation was carried out on the basis of the mathematical model given in [3]. It is known that smoke gun powder (black powder) is often used as an igniter. The peculiarity of such powders is their rapid ignition, high combustion temperature with relatively low caloric content, as well as the content in the combustion products of a significant amount of solid particles K2SO4, K2S, K2SO3, C, etc. Moreover, the condensed phase is 50-60% of the total mass of the combustion products of black powder. The presence of heated particles leads to the appearance of significant heat fluxes to the powder charge surface during their depositions, which are commensurable with convective heat fluxes.

In terms of this mathematical formulation for describing black powder and its combustion products is used a combination of two components of a polydispersed blend of: the actual black powder particle with index \( n \) and formed as a result of its combustion soot index \( l \). It is believed that the combustion of black powder occurs according to the law (8), and the rate of formation of soot particles per unit volume and their mass velocity are determined by the relations

\[
m_{pl} = m_{pn} (1 - c_{gl}) - m_c, \quad u_{pl} = u_n,
\]

where \( c_g \) is mass fraction of the gas formed during combustion of the black powder particle.

Here \( m_c \) is a rate of soot deposition on the surface of the ignited powder element per unit volume, connected with the analogous parameter \( G_c \) from [3] by the relation

\[
m_c = \frac{G_c}{s}
\]

The mathematical model used in comparison with [3] allows to take into account the polydispersity composition of the gas-powder blend, therefore the formulas from [3] should be generalized to this case. Passing from the perimeter of combustion to the bare spot \( s_{pj} \) of the powder element with the index \( j \), this dependence can be represented in the form

\[
G_{cj} = K_0 \frac{\delta \beta_{sl}}{\alpha} \left| u_i - u_j \right|.
\]

In this case, the total velocity of soot mass change due to precipitation in a unit volume will be

\[
m_c = \sum_n G_{cj} = \frac{\delta \beta_{sl}}{\alpha} \sum_n K_0 s_{pj} \left| u_i - u_j \right|
\]
Here the summation is carried out over all indices \( j \) ignited but not yet burning propellant elements. For the sedimentation coefficient \( K_0 \), the same functional dependence is used as in \([3]\).

Assuming that the heat flow is due to convective heat transfer from the relative motion of the gas flow near the powder element and the conductive heat transfer due to the deposition of black powder particles, and adopting the principle of additivity of the heat flow components, we have an expression for the heat flux into the ignited kind \( j \) element

\[ q_j = (\alpha_{c_j} + \alpha)(T - T_{nj}), \]

where \( T \) is gas blend temperature;
\( T_{nj} \) – surface temperature of the ignited powder element.

For the convective heat transfer coefficient we have the known relation

\[ \alpha = \frac{\lambda Nu_j}{d}. \]

Here \( \lambda \) is coefficient of gas thermal conductivity;
\( Nu_j \) – the Nusselt number, known flow conditions function;
\( d \) a characteristic linear dimension, which for a packet of tubes can be represented in the form

\[ d = \frac{4\alpha}{\sum s_j \beta_j}. \]

The expression for the heat flux is used as the boundary condition in the tack of surface igniting of the powder element of grade \( j \) on the basis of a solid-phase ignition model. For each of the igniting, but have not yet burning powder particles to solve the equation

\[ \frac{\partial T_j}{\partial t} = \frac{\lambda}{\delta c} \frac{\partial^2 T_j}{\partial n^2} + \frac{Q}{c} z \exp\left(-\frac{E_a}{RT_j}\right) \]

under the following initial and boundary conditions:

\( T_j(x, n, 0) = T_0; \quad n \geq 0; \)

\[ -\lambda \frac{\partial T_j}{\partial n} = (\alpha_{c_j} + \alpha)(T - T_{nj}); \quad n = 0; \]

\[ \frac{\partial T_j}{\partial n} = 0; \quad n \rightarrow \infty, \]

where \( T_0 \) is initial temperature of propellant.

Equation (10) is solved until the moment of ignition, in which quality the surface of the particle is used to reach a sufficiently high temperature \( T^* \). After that, the particle is considered to be burning and the gas flow from it is calculated by (8).

As an example, figures 1 and 2 show the results of calculations for two tube powders types as 22/1 and 11/1.
Figure 1. Charge ignition time for powder 22/1.

Figure 2. Charge ignition time for powder 11/1.
The times of charge elements ignition for different cross sections of the charge are shown. During these calculations, the black powder mass was significant relative to the main charge mass. As a result, the sections located at the charging chamber bottom are ignited later than in the middle of the chamber. This is explained by the increase of the heat flux in the chamber middle due to the convective component, which depends on the powder gases velocity. Powder with a smaller depth of vault (11/1) ignites faster than 22/1.

Figure 3 shows the results of calculations for a variant more appropriate to the real masses ratios of black powder and the main charge. One igniter was located at the chamber bottom, the second was in the middle of the main charge. A solid curve shows the dependence of the ignition time on the cross section coordinate. A dashed curves and dots represent respectively the values of the integrals

\[ I_{\text{convective}} = \int_{0}^{t_{\text{ign}}} \alpha(T - T_{\text{w})} dt \]
\[ I_{\text{conductive}} = \int_{0}^{t_{\text{ign}}} \alpha(T - T_{\text{w})} dt \]

representing the amount of energy per unit of the surface to be ignited. In this case, the leading mechanism in the process of whole charge ignition is the conductive mechanism due to the deposition of hot particles of black powder. Its role is essential for igniting the part of the charge that is located at the bottom of the charging chamber. Here, the \( I_{\text{conductive}} \) value significantly exceeds \( I_{\text{convective}} \), which determines the short ignition time of the main charge elements located here. Subsequently, the powder gases flowing from the charging chamber bottom increase the convective heat flow and the role of the convective mechanism for igniting the main charge elements located at a distance from the charging chamber bottom is the leading one.

4. Conclusion

In this article, there was described the mathematical model intended to investigate the wide class of internal ballistic processes in high-speed propulsion systems. Its elements and general approach were used in modeling processes in light-gas installations [9]. The implementation in the form of the
software package allowed it to be used by its personnel who are not specialists in the field of mathematical modeling.

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