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Peshkov R. A., Ismagilov D. R.

Numerical simulation of the interaction between combustion products of a cartridge pressure accumulator and oxygen in the launch container

The paper introduces a mathematical model for calculating the gas-dynamic parameters in the launch container. The model takes into account chemical interactions between the main components of the combustion products, i. e. carbon monoxide and hydrogen, and oxygen. The resulting energy can be used to increase the initiating pulse of the rocket. Within the research, we described the basic requirements for the grid model, and analyzed the accuracy of the results obtained. Furthermore, we compared calculation data of pressure in the launch container with the results of the known method. Findings of research show that the use of two-dimensional and three-dimensional models makes it possible to obtain not only medium-volume gas-dynamic parameters, such as pressure, temperature, density, but also the distribution of these parameters over the computational domain. The developed method of numerical simulation will allow us to estimate the effect of changes in the configuration of the sub-rocket volume and other parameters on the dynamics of the rocket movement without conducting an expensive experiment.

Keywords: gas dynamics, modeling, methods, dissociation, recombination

At the launch phase, the main tasks are to make the missile leave the launch container at a predetermined speed and to determine gas-dynamic loads acting upon the structural elements of the launch container and the missile. The loading analysis shall be conducted at the launcher project definition stage before manufacturing full-scale assemblies or when some assemblies and components of the missile and launch container are partly completed. When studying the movement of the missile in the launch container, the main function is to change the sub-missile volume pressure, which determines the dynamics of missile movement in the launch container and the speed at which the missile leaves the container. While previously physical experiment was the main tool for obtaining results, nowadays fast development in computer engineering gives another complementary tool, i. e. numerical experiment that allows to reduce costs of missile launch. There are many methods intended to determine gas-dynamic parameters in the launch container. One of the problems related to the method development is to consider the processes associated with mixing of solid fuel combustion products with cold air. These processes are underexplored, especially the initial stage when the sub-missile volume in the container is being filled. Basically, the complexity of these thermogasdynamic processes is associated with unsteady chemical interaction. To estimate the effect of the unsteady behaviour of thermogasdynamic processes in progress, we carried out calculations using two-dimensional axis-symmetrical and zero-dimensional models.

Thermogasdynamics of variable mass of gas shall be analysed with regard to afterburning of combustible components in the presence of gas phase changes of carbon oxide when high-temperature combustion products of solid propellant charges are mixed with air environment.

Solid propellant charge combustion products contain a considerable amount of carbon oxide (up to 70 %). Carbon oxide along with hydrogen (the content of which in combustion products may reach 3 %) are combustible components and react with atmospheric oxygen within the initial volume of the launch container. In addition to the specified combustible components, solid propellant charge combustion products contain non-combustibles such as carbon dioxide, nitrogen, and water vapours, with the percentage content of each component up to 10 % [1].

In order to estimate the effect of the afterburning processes upon change of medium-volume pressure within the initial sub-missile volume we conducted a calculation, selecting the following parameters of the *Peacekeeper* missile [2] as the initial data: length 21.5 m, diameter 2.4 m,

weight 88,500 kg, container length 24.4 m, container diameter 2.44 m.

Within the scope of numerical experiments the following basic simplifications and assumptions were taken:

• the working medium is a gas mixture, the parameters of which are determined in accordance with the ideal gas law;

• k – ε turbulence model was selected;

• problem solving in axis-symmetrical arrangement;

• launch container's sabot and bottom surfaces are smooth, non-destructible and impenetrable;

• structure walls are adiabatic.

The simulation model is similar to the models described in the research paper [3], but it has its own distinctive features, basically associated with setting up the boundary conditions, selection of a grid model and consideration of processes of interaction between the gas mixture and atmospheric oxygen within the sub-missile volume. Mass flow rate, temperature and pressure were selected as the boundary conditions at the output of the cartridge pressure accumulator [4]. Thermodynamic parameters of solid propellant charge combustion products depend on fuel grades containing various mass fractions of chemical components and, generally, do not have clear cut distinctions. For different operating pressures these parameters can be as follows [1]:

• temperature of 2800 to 3800 K (rarely, it can be equal to 1500 K, for example, for fuels intended for auxiliary applications and experimental testing);

• gas constant of 290 to 330 J/kg·K (rarely, it can reach 400 J/kg·K for fuels intended for auxiliary applications and experimental testing);

• adiabatic exponent of 1.05 to 1.25.

As the boundary conditions were time-dependant, we used special user-defined functions (*UDF*). Impermeability and initial wall temperature were selected as boundary conditions on the wall.

Fig. 1, a, shows the layout of the sabot and propellant gas feed into the volume [4]. Based on the available geometry, we built a two-dimensional grid model symmetrical to the missile axis. Such a problem statement allowed to use a hexahedral grid. A tetrahedral grid can be used, but it requires a larger number of elements to obtain results with the similar accuracy. Grid generation involved grid clustering toward the sabot surface and to the bottom of the launch container in order to calculate boundary layer parameters. To determine the cell height on the

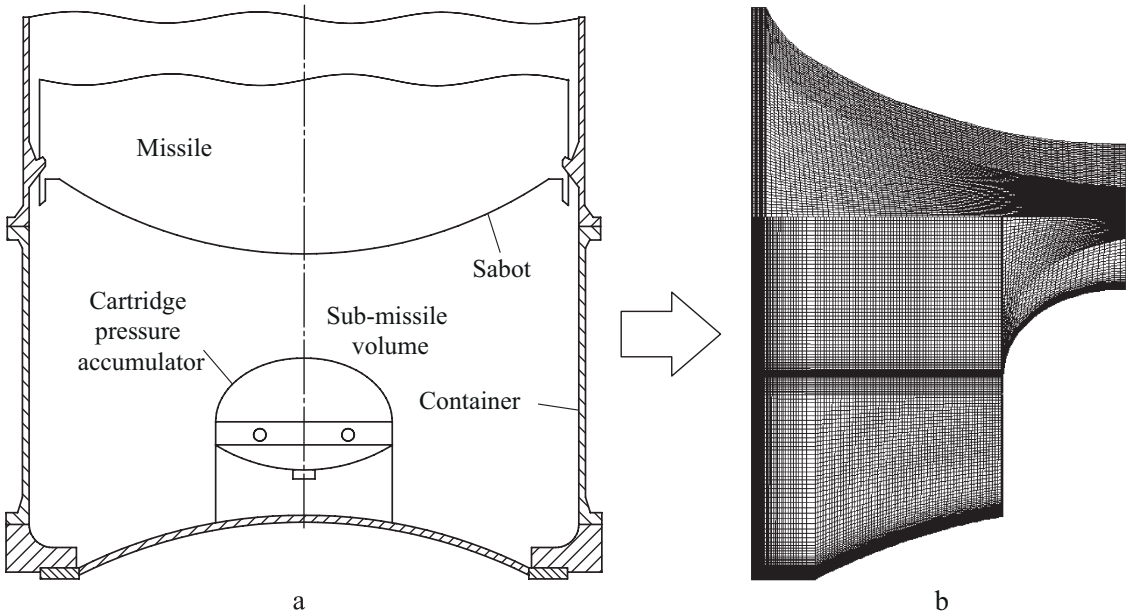

Fig. 1. Grid motel generation stages: a – sabot layout; b – grid model

surfaces, the condition of parameter $y^+ = 30…50$, shall be met as required by the used turbulence model $k - \varepsilon$.

Fig. 1, b, shows the result of grid setup for modelling gas-dynamic processes within the initial volume of the launch container using the developed recommendations.

This paper describes the gas mixture consisting of the following components: N_2, O_2, CO_2, CO, H_2, N_2, H_2O, C, O, H, HO_2, OH, H_2O_2, HCO.

The gas mixture composition and mass fractions in the sub-missile volume at the initial time point are as follows: N_2 – 77 %, O_2 – 23 %.

The composition and mass fractions of combustion products fed from a cartridge pressure accumulator: CO_2 – 10 %, CO – 67 %, H_2 – 3 %, N_2 – 10 %, H_2O – 10 %.

Ideal gas mixture law for compressible flows:

$$\rho = \frac{p_{\text{абс}}}{RT\sum_i \frac{Y_i}{M_{wi}}},$$

where $p_{\text{абс}} = p_{\text{отн}} + p_{\text{изб}}$;

$Y_i = m_i / m$ – mass fraction of the i-th component;

M_{wi} – molecular weight of the i-th component.

Mass transfer equation for each component of gas mixture:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla(\rho \mathbf{V} Y_i) = -\nabla(\mathbf{J}_i) + R_i,$$

where Y_i – local mass concentration of the i-th component;

$\mathbf{J}_i$ – diffusion flow of the i-th component,

R_i – rate of the i-th component formation in chemical reactions.

In the mixture, there are reactions of combustion, dissociation, and recombination which can be represented as follows:

$$\sum_{i=1}^{N_{R_1}} \nu'_{i,\gamma} M_i \overset{k_{f,\gamma}}{\rightarrow} \sum_{i=1}^{N_{R_2}} \nu''_{i,\gamma} M_i,$$

where N_{R_1} – number of reagents;

$\nu'_{i,\gamma}$, $\nu''_{i,\gamma}$ – stoichiometric coefficients;

M_i – character corresponding to the grade of gas mixture;

$k_{f,\gamma}$ – rate constant of the γ-th chemical reaction;

γ – number of reaction;

N_{R_2} – number of reaction products.

Rate of the i-th component formation in chemical reactions R_i:

$$R_i = M_{wi} \sum_{\gamma=1}^{N_R} \hat{R}_{i,\gamma},$$

where M_{wi} – molecular weight of the i-th component;

N_R – number of chemical reactions;

$\hat{R}_{i,\gamma}$ – rate of the i-th component formation/destruction in chemical reaction.

The table represents a structure of applicable chemical transformations and single-temperature constants of reaction rates at the low pressure limit.

List of chemical transformations and single-temperature constants of reaction rates

Reaction	A_f, m^3/kmol·c	β	E_a, J/kmol
$2H_2 + O_2 \leftrightarrow 2H_2O$ (global combustion reaction consisting of 19 elementary reactions) [5]	–	–	–
$2CO + O_2 \leftrightarrow 2CO_2$ (combustion) (global combustion reaction consisting of 17 elementary reactions) [6]	–	–	–
$CO_2 \leftrightarrow CO + O$ (dissociation) [7]	1.7·1028	–4.22	538.8·106
$CO + O \leftrightarrow CO_2$ (recombination) [7]	4·1021	–2.97	31.8·106
$CO \leftrightarrow CO + O$ (dissociation) [7]	1.4·1018	–1.39	1069.3·106

Rate of the i-th component formation/destruction in chemical reaction:

$$\hat{R}_{i,\gamma} = \left(\nu''_{i,\gamma} - \nu'_{i,\gamma}\right)\left(k_{f,\gamma} \prod_{j=1}^{N_{R1}} [C_j]\right),$$

where C_j – molar concentration of the j-th component.

Constants of chemical reaction rates are determined by the Arrhenius law:

$$k_f = A_f T^{\beta} e^{-\frac{E_a}{RT}},$$

where A_f – pre-exponential factor;

β – temperature index;

E_a – activation energy;

R = 8314.46 J/kmol·K – universal gas constant;

T – temperature.

Advanced software packages use residual levels for convergence estimate of the solution. A residual calculated by the solver is the summarized imbalance in equation (1) calculated in all grid cells P:

$$a_P \varphi_P = \sum_{nb} a_{nb} \varphi_{nb} + b, \qquad (1)$$

where a_P – central coefficient;

a_{nb} – coefficients of influence on adjacent cells;

b – contribution of constant component of source term S_c to $S = S_c + S_p \varphi$ and boundary conditions.

Despite the fact that the values of globally scaled residuals were a bit higher than the recommended values at the initial simulation stage, on average, in the course of the analysis of convergence and robustness of calculations during numerical experiments, globally scaled residuals did not exceed 10^{-3} for all the equations, except for the energy equation, for which the residuals were less than 10^{-6}. This result complies with recommendations provided by developers of advanced gas dynamics simulation software packages.

The analysis of the effect of the time interval on the medium-volume pressure at the initial stage of filling the sub-missile volume in the container has proved that a decrease in the time interval by less than 10^{-5} s does not lead to a considerable change of this parameter (Fig. 2). The selected time interval is a recommended value that can be specified as an additional assumption when solving the problem under discussion, because typical duration of chemical processes has not been analysed.

Calculations have been completed before the missile starts to move in the launch container.

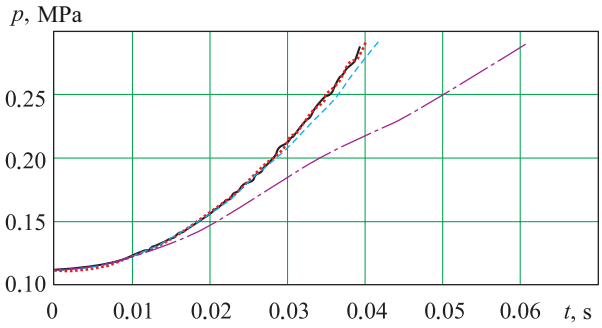

Fig. 2. Change of medium-volume pressure in container for various time intervals: –·– – 1e-03 s; - - - – 1e-04 s; ····· – 1e-05 s; —— – 1e-06 s

This time parameter depends on the required value of displacement pressure:

$$p = \frac{4mg}{\pi d_k^2} + p_h = \frac{88{,}500 \cdot 9.8 \cdot 4}{\pi \cdot 2.44^2} + 101{,}325 = 286{,}900 \text{ Pa},$$

where m – missile weight;

g – gravity acceleration;

d_k – container diameter;

p_h – atmospheric pressure.

At the next stage of problem solving, i. e. the missile movement in the container, it is recommended to reduce the time interval.

We should note that generally residuals are not a generic criterion for estimating correctness of the obtained result, because they indicate only the accuracy of the calculation pattern and mathematical model. At that, even high residual values allow to obtain good results with the required accuracy. That is why this paper also describes comparison with the results obtained by means of a zero-dimensional model.

According to calculation results, we plotted graphs depicting medium-volume pressure variations in the container with and without regard to chemical interaction processes (Fig. 3).

Calculations of gas-dynamic parameters in the launch container at missile launch with the help of the developed numerical simulation method prove that simulation with regard to chemical processes has resulted in a decrease in the missile lift-off time by 15 %. Thus, simulation with regard to chemical transformations is important for calculating the speed and time required for

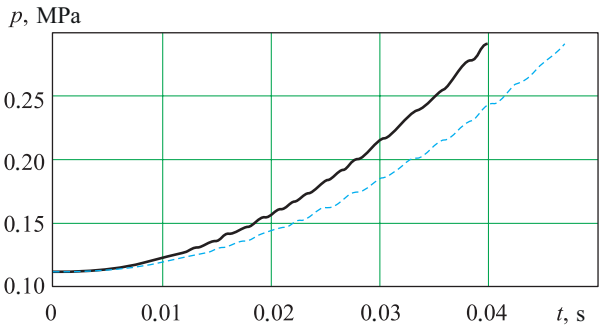

Fig. 3. Change of medium-volume pressure in container:
—— – s with regard to chemical processes;
---- – without regard to chemical processes

the missile to leave the container, which are the key parameters in control system development.

At the initial stage, in order to compare the results obtained, we made calculations using a zero-dimensional model based on the differential equation solution that describes the medium-volume pressure in the launch container (without regard to the processes of recombination, dissociation, afterburning, and gas heat exchange with the container walls and the missile sabot) [1]:

$$\frac{dp}{dt} = \frac{k-1}{V}\left[\frac{k}{k-1}\dot{m}RT\right], \qquad (2)$$

where p – pressure;

k – adiabatic exponent;

V – sub-missile volume;

$\dot{m}$ – mass flow rate of gas per second from cartridge pressure accumulator;

R – initial gas constant.

The energy generated due to heat emission during afterburning of combustible products (carbon oxide and hydrogen) in propellant gases can be expressed through the heating value:

$$dQ_{\text{дог}} = \left(H_{\text{CO}}q_{\text{CO}} + H_{\text{H}_2}q_{\text{H}_2}\right)\dot{m}, \qquad (3)$$

where $H_{\text{CO}} = 283$ kJ/mol – heating value of carbon oxide;

$q_{\text{CO}} = 0.7$ – carbon oxide content in gases fed into sub-missile volume;

$H_{\text{H}_2} = 241.84$ kJ/mol – heating value of hydrogen;

$q_{\text{H}_2} = 0.03$ – hydrogen value in gases fed in sub-missile volume.

Thus, to take into account afterburning of combustion product components, the obtained expression (3) shall be added to the equation (2):

$$\frac{dp}{dt} = \frac{k-1}{V}\left[\frac{k}{k-1}\dot{m}RT + \left(H_{\text{CO}}q_{\text{CO}} + H_{\text{H}_2}q_{\text{H}_2}\right)\dot{m}\right].$$

Calculations of gas-dynamic parameters in the launch container during missile launch using a zero-dimensional model show that the missile lift-off time slightly changed by 4.5 % (Fig. 4) with regard to the energy generated due to heat emission caused by afterburning of combustible components (carbon oxide and hydrogen) in propellant gases.

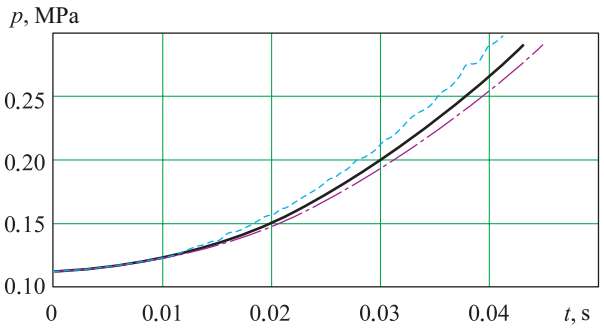

Fig. 4. Change of medium-volume pressure in container:
—— – with afterburning (zero-dimensional model);
---- – with afterburning (two-dimensional model);
–·–· – without afterburning (zero-dimensional model)

As Fig. 4 shows the results obtained without calculation of the reactions of dissociation and recombination, we used a 2D axis-symmetrical model for calculation with regard to afterburning reactions only (first two reactions in the table).

Comparison with a zero-dimensional model allows to make the following conclusion: the difference in the missile lift-off time values is 9 %, taking into account the combustion reaction only. This proves the efficacy of the developed numerical simulation method. The obtained difference in values is probably associated with the condition that the zero-dimensional model has been used regardless of elementary reactions that go along with the global reaction and limited oxygen reserve.

Application of 2D and 3D models allows to calculate not only medium-volume gas-dynamic parameters (pressure, temperature, density), but also the distribution of these parameters within the computational domain. This advantage can be used for solving heat exchange problems (where values

of gas-dynamic parameters near the walls are more important than average values of the parameters) and for determining mass contents of chemical substances in the sub-missile volume. The next phase of the study is numerical simulation of the dynamics of missile extraction out of the container (until the missile bottom leaves the container) with regard to chemical transformations, heat exchange processes, plus an analysis of the effect of various structural parameters (configuration of container bottom and missile sabot, parameters of heat-resistant coating) on the speed and time required for the missile to leave the container.

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Peshkov Ruslan Aleksandrovich – Candidate of Engineering Sciences, Associate Professor, Department of Aircrafts, Federal State Autonomous Educational Institution of Higher Education "South Ural State University (National Research University)", Chelaybinsk.
Science research interests: numerical simulation of the dynamics of the launch, the design of spacecrafts.

Ismagilov Denis Rashidovich – Research engineer, Scientific and educational center "Aerospace technologies", Federal State Autonomous Educational Institution of Higher Education "South Ural State University (National Research University)", Chelyabinsk. Science research interests: numerical simulation of high-speed flight aerodynamics.

Численное моделирование взаимодействия продуктов сгорания порохового аккумулятора давления с кислородом воздуха в пусковом контейнере

Представлена математическая модель расчета газодинамических параметров в пусковом контейнере с учетом химических взаимодействий основных компонентов продуктов сгорания: окиси углерода и водорода с кислородом. Полученная энергия может использоваться для увеличения стартового импульса ракеты. Описаны основные требования, предъявляемые к сеточной модели, и проанализирована точность получаемых результатов. Проведено сравнение данных расчета давления в пусковом контейнере с результатами известной методики. Сделан вывод о том, что использование двухмерных и трехмерных моделей позволяет получать не только среднеобъемные газодинамические параметры (давление, температуру, плотность), но и распределение этих параметров по расчетной области. Разработанная методика численного моделирования позволит оценить влияние изменения конфигурации подракетного объема и других параметров на динамику движения ракеты без проведения дорогостоящего эксперимента.

Ключевые слова: газодинамика, моделирование, методика, диссоциация, рекомбинация.

Пешков Руслан Александрович – кандидат технических наук, доцент кафедры «Летательные аппараты» Федерального государственного автономного образовательного учреждения высшего образования «Южно-Уральский государственный университет (Национальный исследовательский университет)», г. Челябинск.
Область научных интересов: численное моделирование газодинамики старта, проектирование космических аппаратов.

Исмагилов Денис Рашидович – инженер-исследователь научно-образовательного центра «Аэрокосмические технологии» Федерального государственного автономного образовательного учреждения высшего образования «Южно-Уральский государственный университет (Национальный исследовательский университет)», г. Челябинск.
Область научных интересов: численное моделирование аэродинамики высокоскоростного полета.