Modeling of Condensed Combustion Products in a Combustion Chamber

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Abstract: The work is devoted to solution of the problem of condensed combustion products properties prediction at the surface of burning propellant and within multiphase flow. Condensed combustion products characteristics at a surface of burning propellant are determined using decision making system which includes a set of formalized and unformalized procedures that respectively based on mathematical models and experimental regularities. For determining the properties of condensed products in combustion chamber environments, the evolution model was developed with considering of non-uniform flow nature, interactions between agglomerates and gaseous combustion products. The developed models allow determining the condensed combustion products properties depending on propellant formulation, burning conditions, geometric configuration of propellant grain and combustion chamber. Parametric analysis of the models was performed according to combustion chamber environments.

Keywords: condensed combustion products, agglomeration, smoke oxide, multiphase flow, mathematical modeling.

INTRODUCTION

Formation of condensed combustion products (CCP) occurs as a consequence of aluminum usage as metal fuel in solid propellant composition. As a rule, CCP are characterized by presence of two fractions in particles sizes – smoke oxide particles (SOP) and agglomerates. SOP consist of Al_2O_3 with sizes $\sim 0.1 \div 10.0$ μm. Agglomerates consist of Al, Al_2O_3, have a complex structure, and can significantly exceed in size the initial metal particles.

The relevance of study of CCP formation and evolution is caused by significant influence of CCP on intra-chamber processes. These include slag accumulation, specific impulse losses, erosion of ablative materials, pressure oscillations. Herewith, the sizes and mass fraction of agglomerates and SOP, as well as chemical composition and structure of agglomerates are important.

The relevance of the noticed problems led to appearance of a large number of works devoted to simulation of multiphase flows containing agglomerates. These include the papers by J. Dupays, Y. Fabignon et al. [1], T. Shimada et al. [2], A. Attili et al. [3], J.S. Sabnis [4], and others. A significant number of papers devoted to agglomeration process modeling. The papers by A. Gany et al. [5], N. Cohen [6], V.G. Grigoriev et al. [7], V.D. Gladun et al. [8, 9], T.L. Jackson et al. [10], Maggi et al. [11], S. Gallier [12], S.A. Rashkovsky [13], V. Srinivas and S.R. Chakravarthy [14], and others can be noticed. A limited number of works devoted to modeling of SOP formation. Some aspects of this process are considered in papers by A.N. Zolotko, N.I. Poletaev et al. [15], A.Ya. Lukin, A.M. Stepanov et al. [16], Karasev V.V. et al. [17], and some others.

By the present time, a number of the models allowing determining CCP properties have been developed by authors of the present paper. These include a model of agglomeration at the surface of burning propellant [18, 19], a model of evolution of agglomerates [20] and SOP [21, 22] within the multiphase flow. Also the decision making system about CCP properties which is based on expert system ideology is been developed. The main feature of these models is the ability to calculate not only sizes and mass fraction of CCP but also chemical composition and structure parameters.

In the present paper, the principles of the previously developed models [18-23] usage at intra-chamber conditions are considered. The main features of CCP evolution within combustion chamber are multidimensional nature of multiphase flow, distributed inflow of combustion products, mutual influence of agglomerates evolution and properties of ambient gas phase.

1. PHYSICAL BASIS FOR DESCRIBING THE FORMATION AND EVOLUTION OF CCP

Formation of CCP takes place within the surface layer and on the surface of burning propellant.

Agglomeration takes place in consequence of a *skeleton layer* (SL) formation. Within SL and in its surface, the melting and ignition of initial metal particles is carried out. This leads to the particles coalescence, oxide accumulation and agglomerates formation. In turn, formation of SL is connected with presence of the pockets and inter-pocket bridges (IPB) in initial propellant structure. The pockets are

enclosed between several oxidizer particles while IPB are located within thin layer between two adjacent oxidizer particles [18]. As a rule, SL formation is carried out within the pocket region. In case of usage of oxidizer with relatively low melting temperature the spreading over the propellant surface of oxidizer is possible i.e., loss individuality of oxidizer particles. In this case, the formation of SL becomes possible also within IPB.

In accordance with the pockets conception, each agglomerate can be formed as a result of one pocket (pocket agglomeration mechanism), several pockets (inter-pocket mechanism) or less than one pocket (pre-pocket mechanism) burnout [18].

In case of SL absence, the metal particles leave the propellant surface without agglomeration.

Formation of the SOP is caused by realization of various processes:

- Condensation of products of gas-phase (vapor-phase) combustion of agglomerating metal at propellant surface;
- Condensation of products of gas-phase (vapor-phase) combustion of non-agglomerated metal;
- Oxide accumulation on the surface of burning non-agglomerated metal particles (primarily in the heterogeneous reaction) and their possible fragmentation.

Presence of several mechanisms of SOP formation explains the multimode size distribution of SOP near burning propellant surface.

Within a multiphase flow, the *evolution of CCP* is carried out resulting in formation of final combustion products. The evolution is understood as a set of

physical and chemical phenomena that lead to changing of sizes, chemical composition, structure and mass fraction of CCP. Interactions between fine and coarse fractions of CCP lead to redistribution of their mass fractions and changes in particles sizes. Agglomearates Al combustion leads to changes in properties of gaseous combustion products. Thus, evolution of fine and coarse fractions of CCP as well as gaseous phase is carried out. As a result of the evolution, the final coarse and fine fractions of CCP are formed (Fig. 1).

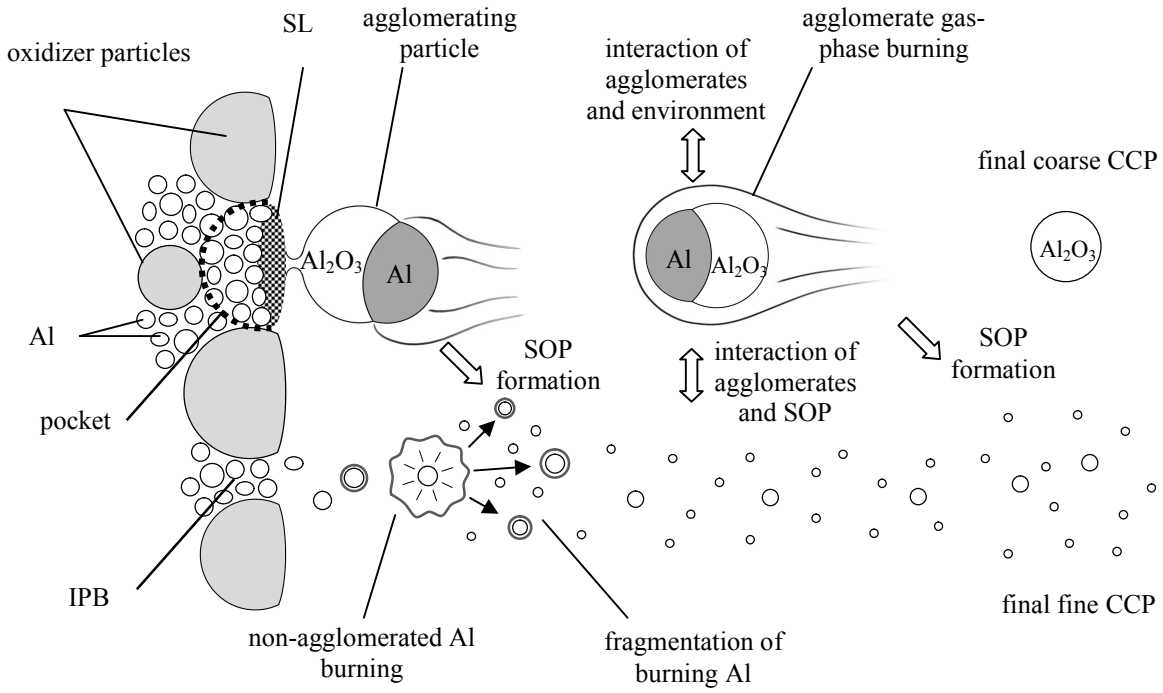


Fig. 1. Scheme of CCP formation and evolution

2. CALCULATION OF CCP PARAMETERS AT PROPELLANT SURFACE

The agglomeration model [18, 19] can be used to determine the properties of emerging agglomerates at burning propellant surface. The model allows determining the following main agglomerates characteristics:

- $f_m(D)$ – mass function of size distribution density of agglomerates;
- D_{43} – mass-medium size of agglomerates, μm;
- Z_m^a – fraction of initial metal used to form agglomerates;
- η – mass fraction of Al_2O_3 in agglomerates;
- Parameters of agglomerates structure.

Scope of the model use is presented in the table 1. The model allows determining or estimating of agglomerates parameters if propellant type and therefore agglomeration regularities are known. Input data of the model are the type and mass fraction of propellant components, sizes of oxidizer particles in propellant, operating conditions (pressure, acceleration).

Under the uncertainty of information about agglomeration regularities, parameters of agglomerates can be determined (or estimated) using decision making system based. The system is based on expert systems ideology and uses the knowledge base [23]. The system allows estimating the properties of a whole set of CCP including agglomerates and SOP. Correctness of the estimation is provided by information content of the knowledge base which includes experimental data and formalized models.

Table 1. Scope of the agglomeration model use [19]

№	SL formation	Keeping of oxidizer individuality	Pressure (P) and agglomeration mechanism	Determining agglomerates parameters
1.	Within all pockets	Full	P < ~1.0 MPa – pocket	$f_m(D)$, Z_m^a, η, agglomerates structure
2.	Within all pockets	Full	P < ~1.0 MPa – pocket	Z_m^a, η, agglomerates structure, upper estimation of D_{43}
3.	Within only pockets that are formed by keeping individuality oxidizer particles	Partial	P < ~4.0 MPa – pocket and inter-pocket, P > ~4.0 MPa – pocket	$f_m(D)$, Z_m^a, η, agglomerates structure
4.	Within all pockets	Full	P < ~0.5÷6.0 MPa* – pocket and inter-pocket, P > ~0.5÷6.0 MPa* – pocket	$f_m(D)$, Z_m^a, η, agglomerates structure

* – The boundary pressure depends on propellant burning rate

3. CALCULATION OF CCP PARAMETERS WITHIN MULTIPHASE FLOW OF COMBUSTION PRODUCTS

Evolution of agglomerates. The model of agglomerates evolution [20] can be used for calculation of agglomerates parameters within multiphase flow. The model

is based on the description of following phenomena:

- Burning of Al in gas-phase mode;
- Chemical interaction between condensed Al and Al_2O_3 resulting in formation of gaseous products;
- Agglomerates structure changes;
- Coagulation of agglomerates and SOP;
- Agglomerates motion within the flow.

Agglomerates evolution simulation is carried out by integrating of the ordinary differential equations describing motion and changes in parameters of single agglomerates at time. The model allows determining the changes in agglomerates parameters from the moment of agglomerates detachment from propellant surface until they hit the chamber walls or enter into a nozzle.

Evolution of SOP. Modeling of SOP evolution is carried out by use of the model [21, 22]. According to the model, SOP are enlarged within gas-phase burning zone of agglomerated Al through condensation of Al combustion products (sub-oxides of dissociated Al_2O_3) on the SOP. The initial SOP are considered as the condensation nuclei. The main assumptions are: condensation is relatively quick, condensation regime is heterogeneous, condensation zone thickness and sub-oxides flux is provided by agglomerates Al gas-phase (vapor-phase) burning model [20], SOP coagulation is determined by Brownian motion, spatial position of condensation zone is determined by gas flow field in the vicinity of the agglomerate. Model is represented by a system of ordinary differential equations describing changes of the mass and number of particles of each fraction of SOP sizes due to coagulation and condensation processes within an agglomerate Al burning zone. The model uses size

distribution function of condensation nuclei as input data. The model allows determining the changes of SOP sizes distribution function in multiphase flow.

4. MODELING OF CCP EVOLUTION IN A COMBUSTION CHAMBER

Modeling of CCP evolution in a combustion chamber is connected with solving of a set of problems devoted to simulation of a gaseous phase flow, determining of combustion products mixture parameters, calculation of agglomerates and SOP parameters, description of mutual influence of agglomerates, SOP and environments. The accepted approaches for solution of these problems are described below.

4.1. Modeling of Gaseous Phase Flow

Numerical simulation of gaseous flow is carried out by solving the steady-state Navier-Stokes and continuity equations of uncompressible viscous fluid:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \mu\nabla^2\mathbf{u} - \nabla P + \mathbf{f}, \quad (1)$$

$$\nabla\mathbf{u} = 0, \quad (2)$$

where $\mathbf{u}$ – velocity vector, m/s; P – pressure, Pa; ρ – density, кг/м^3; $\mathbf{f}$ – volumetric forces vector, N/m^3, μ – dynamic viscosity, Pa·s. Gas properties are assumed to be a constant. The flow is assumed to be laminar and axisymmetric. In this way, the gaseous phase velocity and pressure fields are determined in cylindrical coordinate system (r, z), where r – radial coordinate, and z – longitudinal coordinate.

Boundary conditions are determined by geometric parameters of calculation domain, mass flux of gas supply, and pressure in outlet region. Mass flux (kg/m^2/s) of gas supply at propellant surface is determined by gasification of propellant components:

$$m_{\mathrm{g}} = u_{\mathrm{p}} \left\{ 1 - Z_{\mathrm{m}}^{\mathrm{p}} \left[\frac{2\mu_{\mathrm{Al}} + 3\mu_{\mathrm{O}}}{2\mu_{\mathrm{Al}}} \left(1 - Z_{\mathrm{m}}\right) + Z_{\mathrm{m}} \right] \right\} \Big/ \sum_n \frac{z_n}{\rho_n}, \qquad (3)$$

где u_{p} – linear burning rate of propellant grain, m/s; $Z_{\mathrm{m}}^{\mathrm{p}}$ – mass fraction of Al in propellant; μ_{Al}, μ_{O} – molar masses of elements Al and O, kg/mole; Z_{m} – ratio between unburned Al in agglomerates and initial Al in propellant; z_n, ρ_n – mass fraction and density of *n*-th propellant component. Pressure in outlet section is determined by operating conditions.

4.2. Discretization of Computational Domain

Discretization of computational domain is needed in order to further description of interactions between agglomerates, SOP, and gaseous phase properties. The discretization is performed by creation of curved mesh connected with streamlines of gaseous phase flow. A cell of such mesh is represented by a stream tube. Within the each *k*-th cell, a curvilinear coordinate system is constructed. Axis of such coordinate system (s_k) is coincident with a streamline. Origin of the coordinate system corresponds to the surface of propellant grain.

Further, the parameters of agglomerates, SOP, and gaseous phase are determined as functions of s_k within each *k*-th cell. Interpolation of the functions

values between cell axes allows determining field parameters in cylindrical coordinates (r, z).

4.3. Determination of Agglomerates Parameters

The agglomerates parameters are determined using the discrete trajectory approach. According to this, the agglomerates phase is represented by set of discrete particles. The problem of agglomerates evolution modeling is solved by calculation of agglomerates trajectories and determining of agglomerates parameters along the trajectories. Herewith, the continuous function $f_{\mathrm{m}}(D)$ is sampled for a several fractions with agglomerates sizes D_i and corresponding mass fractions z_i, where i – fraction number. Propellant surface is sampled for a several fragments from which agglomerates of all fractions are injected. Thus the mass flow (kg/s) of agglomerates of i-th size fraction from j-th propellant fragment is determined by equation:

$$M_{\mathrm{a}i,j} = u_{\mathrm{p}} \cdot \rho_{\mathrm{p}} \cdot Z_{\mathrm{m}}^{\mathrm{p}} \cdot Z_{\mathrm{m}}^{\mathrm{a}} \cdot z_i \cdot F_j \left[1 + \frac{3\mu_{\mathrm{O}} \cdot \eta}{2\mu_{\mathrm{Al}} + 3\mu_{\mathrm{O}} \cdot (1-\eta)} \right], \qquad (4)$$

where ρ_{p} – propellant density, kg/m^3; F_j – area of j-th propellant fragment, m^2.

Resulting from evolution modeling the dependencies of agglomerates parameters including coordinates on time for each i,j-th agglomerate (of i-th size fraction injected from j-th propellant surface fragment) are obtained. Then analysis of agglomerates trajectories is carried out. While agglomerate appears within k-th cell, the projection of its parameters on corresponding curvilinear axis s_k is performed.

Thus, parameters of each *i,j*-th agglomerate are determined as functions of curvilinear coordinates s_k within each *k*-th cell.

Dependencies of agglomerates parameters D_{43}, η on s_k are determined by equations:

$$D_{43}(s_k) = \sum_i \sum_j M_{\mathrm{a}\,i,j}(s_k) \cdot D_{i,j}(s_k) \Big/ \sum_i \sum_j M_{\mathrm{a}\,i,j}(s_k), \quad (5)$$

$$\eta(s_k) = \sum_i \sum_j M_{\mathrm{a}\,i,j}(s_k) \cdot \eta_{i,j}(s_k) \Big/ \sum_i \sum_j M_{\mathrm{a}\,i,j}(s_k), \quad (6)$$

where $M_{\mathrm{a}\,i,j}(s_k)$, $D_{i,j}(s_k)$, $\eta_{i,j}(s_k)$ – mass flow, size and oxide fraction of each *i,j*-th agglomerate depending on s_k.

4.4. Determination of SOP Parameters

Modeling of SOP evolution is performed using the approach of one-dimensional flow (quasi-one-dimensional flow within curvilinear stream tube). Herewith, the characteristic length (L_{inv}) of a stream tube is introduced. L_{inv} corresponds to an interval where entire SOP from beginning of this interval is involved in the evolution. Value of L_{inv} depends on gas velocity, mean relative velocity of agglomerates, and summary area of agglomerates midsections in a volume unit.

During modeling the axis s_k within each *k*-th cell is divided on segments with length L_{inv}. At the ends of the segments the mass function of size distribution and mass-medium size ($d_{43\mathrm{sop}}$) of SOP are calculated using the model [22]. It is assumed that between the points the parameters of SOP are changing linearly. Thus, the parameters of SOP are determined as functions of s_k within each *k*-th cell.

4.5. Calculation of Parameters of Combustion Products Mixture

As individual components of the mixture, the 22 species including compounds of elements C, H, O, N, Cl, Al are considered. The mixture parameters are calculated assuming thermodynamic equilibrium state of gaseous and condensed products excluding unburned Al in agglomerates. The evolution of agglomerates leads to decrease of fraction of unburned Al in agglomerates and to increase of Al combustion completeness. The combustion completeness of Al is characterized by parameter X_{m} – ratio between mass of burnt Al and mass of initial Al within the considering computational cell. It allows representing the mixture parameters (temperature, composition, mass and heat transfer properties) as functions of parameter X_{m}.

Within the k-th computational cell the function $X_{\mathrm{m}}(s_k)$ is determined by equations:

$$X_{\mathrm{m}}(s_k) = 1 - Z_{\mathrm{m}} + \sum_i \sum_j \left(M^0_{\mathrm{m}i,j} - M_{\mathrm{m}i,j}(s_k) \right) \Big/ M_{\mathrm{m}k}\,, \tag{7}$$

$$M_{\mathrm{m}i,j} = (1 - \eta_{i,j}) M_{\mathrm{a}i,j}\,, \tag{8}$$

$$M_{\mathrm{m}k} = u_{\mathrm{p}} \cdot \rho_{\mathrm{p}} \cdot Z^{\mathrm{p}}_{\mathrm{m}} \cdot F_k\,, \tag{9}$$

where $M^0_{\mathrm{m}i,j}$ – mass flow of unburned Al of i,j-th agglomerate at entry into k-th cell, kg/s; F_k – propellant surface area in the base of k-th cell, m^2. Determination of temperature and oxidizing potential (molar fractions of Al oxidizing components – mostly H_2O, CO_2 in intra-chamber environments) is important for agglomerates evolution modeling. Dependencies of temperature and oxidizing potential on X_{m} are presented on Fig. 2 for propellants with $Z^{\mathrm{p}}_{\mathrm{m}} = 0.2$ and $Z^{\mathrm{p}}_{\mathrm{m}} = 0.24$ at pressure 6.0 MPa

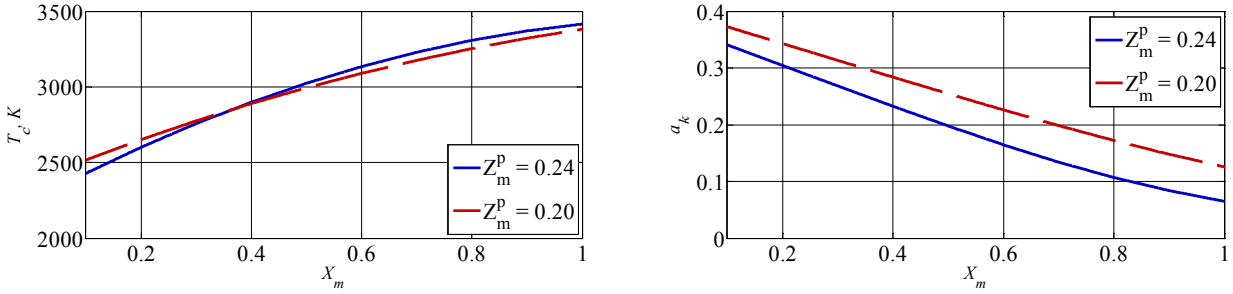


Fig. 2. Dependencies of temperature (T_c) and oxidizing potential (a_k) on X_m for two propellants at pressure 6.0 MPa

4.6. Calculation performing

The calculation continues through global iterations on which sequential recalculations of the fields of gaseous phase and agglomerates parameters are performed. The calculation ends at achievement of required accuracy of X_m at several control points within computational domain. Modeling of SOP evolution is performed on the last global iteration due to weak influence of SOP properties on agglomerates and gaseous phase parameters.

5. MODELING RESULTS

A parametric analysis of developed models was performed applying to a combustion chamber with axisymmetric shape of propellant grain. Geometric parameters of the grain corresponded to the beginning of the working (case I) and intermediate stage on which the half of initial propellant grain depth had burned out (case II), Fig. 3. Chamber pressure was 6.0 MPa in both cases.

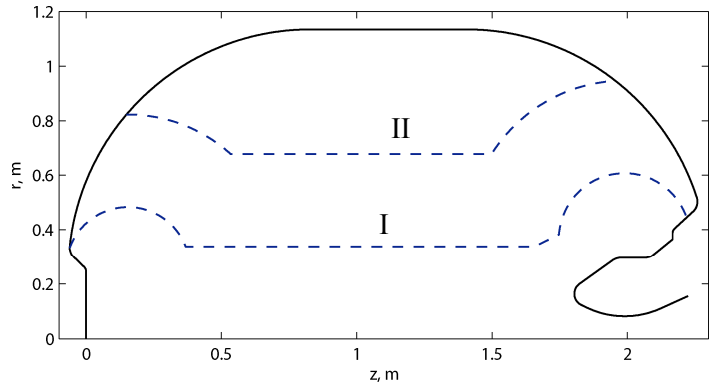


Fig. 3. Combustion chamber and propellant grain geometric configuration in two cases

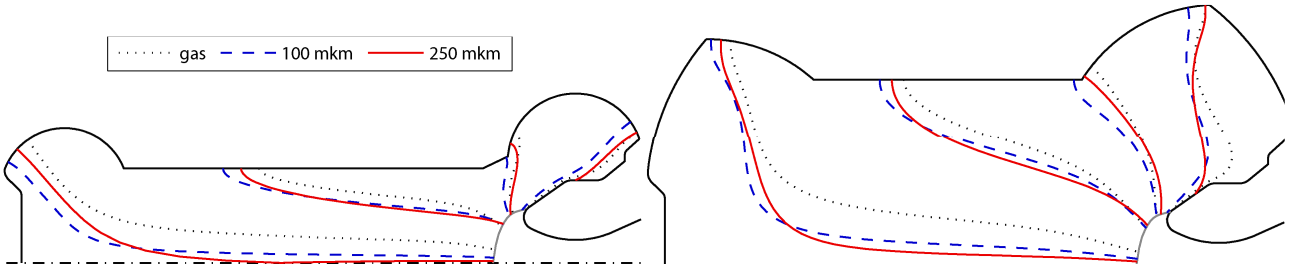
For the estimation of influence of initial CCP parameters, the two propellants with significantly different CCP properties were considered, table 2. In the table values of Z_m^p, values of mass-medium size of initial oxidizer particles (D_{43ox}), values of u_p at pressure 6.0 MPa, and values of D_{43}, η, Z_m^a are presented according to the paper data [24, 25] as well as values of mass-medium initial SOP size (d_{43sop}) are presented according to the paper data [22].

Table 2. Parameters of propellants and CCP

N	Z_m^p	D_{43ox}, μm	u_p, mm/s	D_{43}, μm	η	Z_m^a	d_{43sop}, μm
1	0.20	175	9.82	97	0.34	0.19	0.54
2	0.24	500	8.10	250	0.40	0.34	0.80

On Fig. 4, the stream lines of gaseous phase and trajectories of agglomerates with initial sizes 100 μm and 250 μm are presented. From these results it can be seen

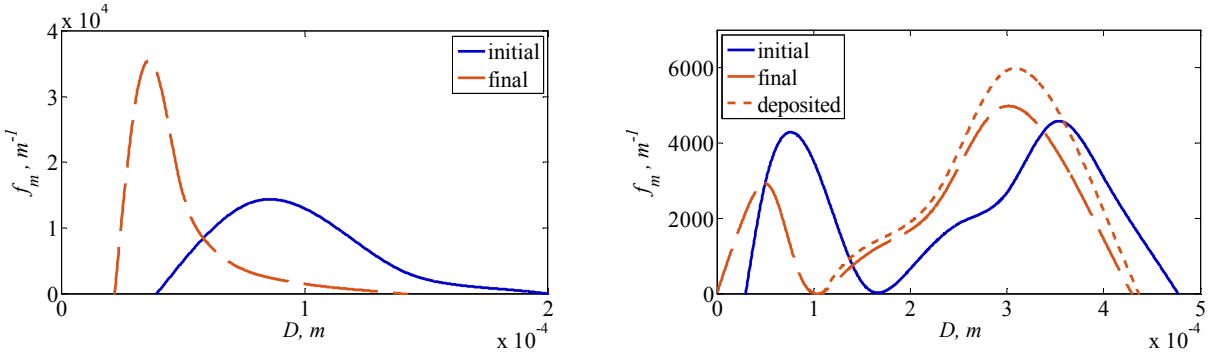
that deposition of coarse agglomerates takes place on the outer surface of submerged nozzle.



Case I Case II

Fig. 4. Gas streamlines and trajectories of agglomerates with initial sizes 50μm and 250 μm

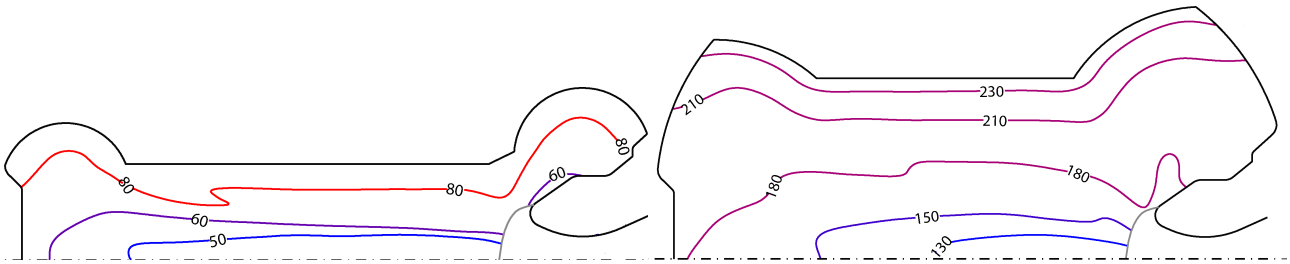
On Fig. 5, the mass functions of size distribution density of agglomerates for both propellants are presented. The functions correspond to agglomerates at propellant surface (initial), at outlet section (final), and deposited on the chamber walls (deposited).



propellant N 1 propellant N 2

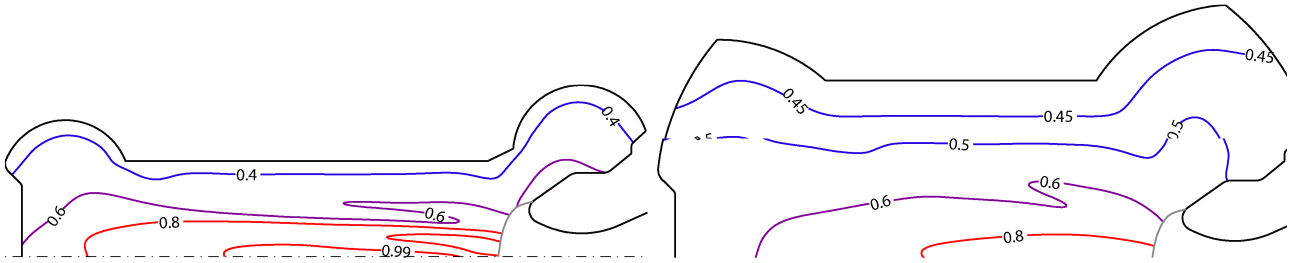
Fig. 5. Size mass density distribution function of agglomerates, case II

Fields of agglomerates parameters D and η with initial sizes 100 μm and 250 μm (correspond to mass-medium sizes of agglomerates for both propellants) are presented on Fig. 6, 7.



case I, propellant N 1 case II, propellant N 2

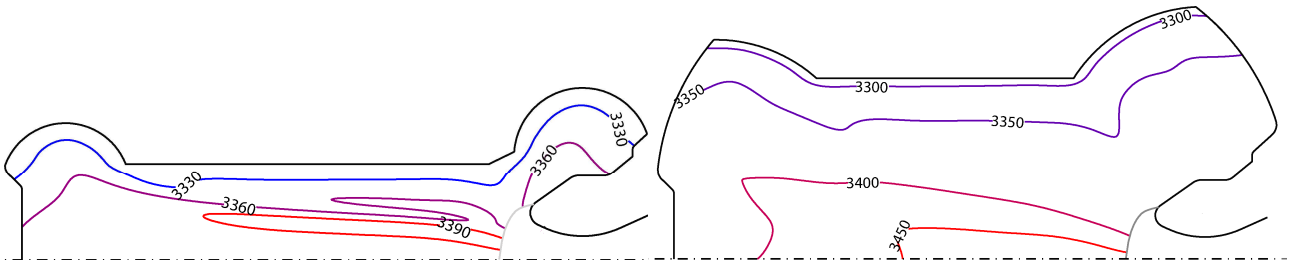
Fig 6. Fields of agglomerates sizes with initial sizes 100 μm and 250 μm



case I, propellant N 1 case II, propellant N 2

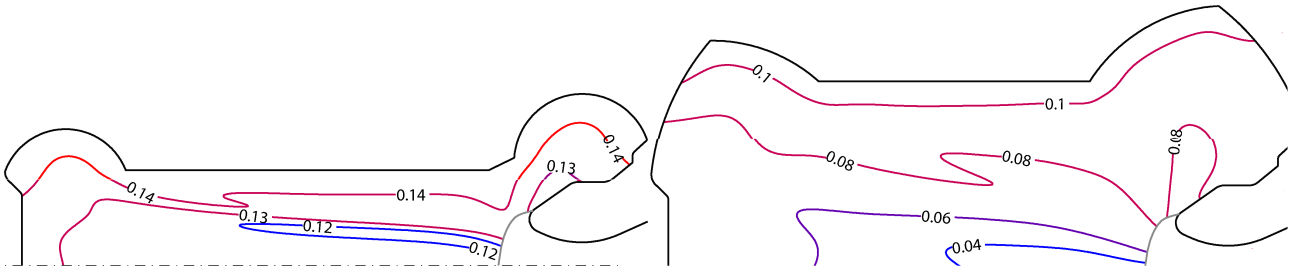
Fig. 7. Fields of parameter η of agglomerates with initial sizes 100 μm and 250 μm

Fields of temperature and oxidizing potential of gaseous phase are presented on Fig. 8, 9.



case I, propellant N 1 case II, propellant N 2

Fig. 8. Fields of gaseous phase



case I, propellant N 1 case II, propellant N 2

Fig. 9. Fields of oxidizing potential

Thus, modeling results allow making conclusions about CCP sizes in various regions of combustion chamber, completeness of metal combustion, slag accumulation. Correctness of obtained results is provided by usage of the models [20, 22] which were verified using experimental data.

CONCLUSIONS

In the present work, the aspects of developed models usage for calculation of CCP parameters were considered. The method for calculation of CCP within axisymmetric multiphase flow with considering of interactions between agglomerates and gaseous combustion products is described. The parametric analysis was carried

out, and its results allowed to make a conclusion about capability of developed models to calculate CCP parameters in intra-chamber conditions.

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