Model of Heterogeneous Condensed Systems Microstructure and Problem of Agglomeration Process Description

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Abstract

A developed model of microstructure of a heterogeneous condensed system is considered in the present paper. The model allows determining parameters of structural formations which are the "pockets" and "inter-pocket bridges". It is shown that modeling results can be used for description of agglomeration – one of the phenomena of burning process. The results were used for estimation of parameters of agglomerates for a number of types of heterogeneous condensed systems. Comparison of calculated and experimental data was carried out. The main regularities are represented rather accurately that evidences on high quality of the model for the description of agglomeration process.

Nomenclature

Roman symbols
Z_{ox} – mass fraction of oxidizer particles in HCS
$Z_{ox'}$ – mass fraction of "minor oxidizer" particles in HCS
Z_p – mass fraction of "pockets" in composition that is considered as homogeneous
$Z_{b\text{-}m\text{-}ox'}$ – mass fraction in propellant of composition that is considered as homogeneous
Z_m^{a} – fraction of initial metal used to form agglomerates
D_{43}^{ox} – mass-medium diameter of oxidizer particles
D_{ox}^{min} – minimum size of oxidizer particle that can form "pockets" and "inter-pocket bridges"
D_{43}^{p} – mass-medium diameter of "pockets"
D_{43}^{a} – mass-medium diameter of agglomerates
V^{Σ}_{ox} – summary volume of oxidizer particles
V^{Σ}_{IPB} – summary volume of "inter-pocket bridges"
V_{ox}^{bas} – volume of single basic oxidizer particle
V_{ox}^{IPB} – volume of single oxidizer particle that forms with a basic particle an "inter-pocket bridge"
P – pressure
l_{ji} – distance between j-th basic particle and i-th surrounding particle
$f_m(D)$ – mass function of size distribution density
k – coefficient of matching

Greek symbols
ρ_{ox} – oxidizer density
$\rho_{b\text{-}m\text{-}ox'}$ – homogeneous matrix density
θ_{Σ} – summary solid angle that is formed by surrounding particles with the basic one

Acronyms
HCS – heterogeneous condensed system
IPB – "inter-pocket bridge"
SL – skeleton layer

1. Introduction

Heterogeneous condensed systems (HCS) are the mixtures of fuel and oxidizer components, in where solid particles of the dispersed phase (mainly metal fuel and oxidizer) are kept together by a homogeneous binder. As a metal fuel the aluminum is widely used. The particles dimensions can vary widely – from a part of micrometer to hundreds micrometers. HCS have the isotropic macroscopic properties due to a random arrangement of particles. Nevertheless there is no doubt that the microscopic structure inhomogeneities affect on the physical and mechanical properties of HCS as well as on their burning process. Therefore a development of an adequate model of the microstructure of HCS is quite important. Microstructure description should be put in base of agglomeration process description as well as the burning process description in the whole.

In the present paper we consider a method for modeling of microstructure of HCS and usage of the modeling results for description of one of the phenomena of burning process – the agglomeration process (enlargement of condensed combustion products in surface layer of burning HCS).

Various existent approaches for modeling of heterogeneous materials microstructure were considered. A large group of the methods is presented by models that perform a packing procedure of a set of solid particles within some representation volume of the material. Therefore a random arrangement of solid particles is represented. In this case the requirement of particles non-overlapping as well as preserving of initial components content and their distributions is important. Furthermore a question of type of the distribution law of particles centers appears to be significant in case of presence of loose packs.

A method based on Lubachevsky and Stillinger ideas [1] is widely spread. The main feature of such method is description of moving, colliding and growing solid particles. Based on this method a set of microstructure models of HCS was created [2 – 5]. The specifity of such models is a description of the most dense packings of solid particles. It should be noted that for real HCS the maximum packing density is not achived due to reduction of mechanical properties of HCS.

A model [6] is based on description of moving particles centers like the moleculas in a gas. The pushing force is considered for ensure the particles non-overlapping condition.

Another group of methods is based on random placing of stationary particles. The particles can be placed all together [7] or added sequentially one by one checking the presence of overlaps [8 – 9]. In [8] packing procedure is performed on two-dimentional planes which simulate slices of HCS.

A few agglomeration numerical models were proposed basing on various interpretations of microstructure modeling results. In [8, 10] the radial distribution function analysis allow identifying of “pockets” and determining of characteristic size of agglomerates. However obtaining of radial distribution function only does not allow determining of size distribution and fraction of agglomerates. In [11, 12] a proximity criterion of adjacent metal particles is used for agglomerate formation description. Such model allows determining a size distribution function of agglomerates as well as their fraction relative to initial metal content. Also a model [13] allows determining such parameters based on identification of congestions of initial particles of metal in HCS.

Besides of microstructure analysis in papers [10, 12, 14 – 16] an influence of various phenomena of burning propellant is considered for modeling of agglomeration. In particular the propellant burning rate, aerodynamic lifting force [14], temperature and distribution of oxidizer flames on the burning surface [15, 16] are taken into account as factors affecting on agglomeration process.

In general outlined above microstructure interpretations appear to be deficient for agglomeration process description. The question of correct usage of the models above remains opened. The described situations are not universal and often do not correspond to the experimentally observed regularities. In particular the metal particles proximity criteria [11, 12] are applied for specific formulations of HCS and do not represent the general regularities of agglomeration process. The formation of metal clusters [14] is not necessary condition for possibility of the agglomeration process realization. The breakaway of agglomerates criterion that related to metal ignition [15] contradicts the experimental data for most types of HCS.

The present model of the structure of HCS is based on ideas outlined in [17]. The main feature of the model is absence of real three-dimensional microstructure representation. Instead the sizes and distances between adjacent oxidizer particles are simulated. Thus the parameters of local structural formations are determined. It allows estimating the size distribution of agglomerates and a fraction of agglomerated metal relative to initial metal content in certain conditions. The modeling results were compared with experimental data for various types of HCS. The main regularities are represented rather accurately that evidences on adequacy of the model. The model takes into account the features of loose or jammed packs of oxidizer particles. It is shown that the model can be used as a part of instruments for definition of characteristics of the condensed combustion products.

2. The Model Description

In the present work the conception of *“pockets”* and *“inter-pocket bridges”* (IPB) is used for the structure description. A “pocket” consists of metal particles, “minor oxidizer” particles and binder. A “pocket” appears between several coarse oxidizer particles. IPB is a part of “metal fuel – minor oxidizer – binder” composition that enclosed between two adjacent oxidizer particles. According to this approach microstructure of HCS can be represented by oxidizer particles, “pockets” and IPBs (Figure 1). It should be noted that so-called “minor oxidizer” particles are the part of fine oxidizer fraction that is considered as a part of homogeneous matrix in HCS. The sizes of “minor oxidizer” particles are comparable with metal particles sizes.

Empirical relationships and coefficients are applied for the identification of “pockets” and IPBs. Values of the coefficients are obtained by the results of heterogeneous material slices analysis [17]. A possibility of presence of smaller structural formations within bigger “pockets” should be taken into account. The model provides determination of size distribution function of the “pockets” and their fraction in composition of HCS.

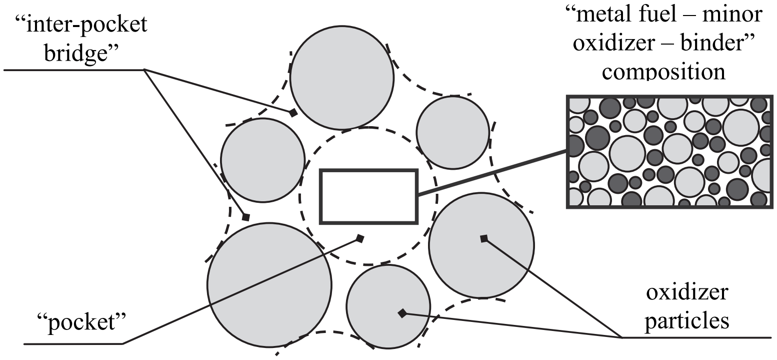


Figure 1: HCS microstructure layout

Let's consider main principles of the model:

- The Monte Carlo method is used. The quantity of centers of particles is distributed under the modified law of Poisson. The distance between two adjacent particles is determined according to mentioned law. Correction of the distance is performed if the particles overlap, i.e. modification of initial Poisson law.
- A planetary model is used for description of local structure around basic particles (Figure 2). Results of the analysis of the surroundings of a large number of basic particles allow to tell about characteristics of HCS in a whole. A number of basic particles should be high enough for represent initial oxidizer particles distribution.

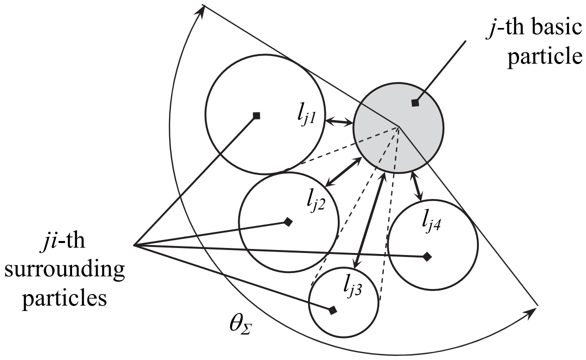


Figure 2: A planetary model of local area in HCS

- A "pocket" is formed by commensurable oxidizer particles. In turn a size of "pocket" is comparable with sizes of oxidizer particles. Shape of "pockets" is considered to be spherical. Identification of "pockets" and IPBs is performed basing on regularities, obtained in [17].
- The sizes of oxidizer particles that form "pockets" and IPBs should be not less than parameter D_{ox}^{min}. Below this size the structure can be considered as homogeneous. Oxidizer particles with the sizes $D_{ox} < D_{ox}^{min}$ are considered as a part of homogeneous matrix. We call them "minor oxidizer". As a rule "minor oxidizer" is a part of fine oxidizer.
- The shape and volume of IPB is defined from Figure 3. IPB volume is limited by surfaces of oxidizer particles and by imaginary surfaces of "pockets".

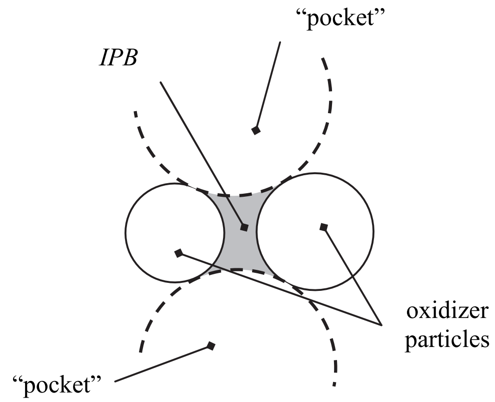


Figure 3: The shape of an "inter-pocket bridge"

Let's explain the used schematization. The planetary model allow determining the distances l_{ji} between basic and surrounding particles only (see Figure 2). Plasing of surrounding particles is performed until summary solid angle that is formed by surrounding particles with the center of basic one (θ_Σ) reaches the value of full solid angle. Using the regularities from [17] the "pockets" and IPBs can be identified and their sizes can be determined. Herewith the relative positions of surrounding particles do not matter due to limitations of planetary model.

While analyzing the local microstructure a direct determination of fraction of "pockets" in HCS is not possible due to the following reasons:

- It is not known exactly how many oxidizer particles (and thus IPBs) form each "pocket";
- Each oxidizer particle that forms a "pocket" can be selected as basic. Thus one "pocket" can be determined by several times.

But the problem can be solved if the fraction of IPBs is determined. Unlike the "pockets" each IPB is formed by two adjacent oxidizer particles only, and fraction of IPBs can be calculated. According to used conception the composition "metal fuel-binder-minor oxidizer" includes "pockets" and IPBs only. Thus the fraction of "pockets" in "binder-metal-minor oxidizer" (Z_p) composition can be determined though the summary volumes of IPBs and oxidizer particles by the following expression:

$$Z_p = 1 - \frac{V_{IPB}^{\Sigma} \rho_{b-m-ox'} (Z_{ox} - Z_{ox'})}{V_{ox}^{\Sigma} \rho_{ox} Z_{b-m-ox'}} \qquad \textbf{(1)}$$

Summary volume of oxidizer particles is determined like a sum of volumes of surrounding and basic particles that form IPBs:

$$V_{ox}^{\Sigma} = k \sum_j V_{ox}^{IPB} + \sum_i V_{ox}^{bas} \qquad \textbf{(2)}$$

The reason of introducing of coefficient k is as follows. While analyzing the local microstructure a possibility of "pockets" and IPBs formation between surrounding particles is not taken into account. Moreover the surrounding particles can belong to structural formations outside the considered local microstructure. In addition the obvious simplification should be noted when the shape of IPB was defined. For compliance with initial ratio between components in HCS the evaluated summary volume of surrounding particles must be restricted by coefficient k. The value of k was determined by performing of minimization of discrepancy between calculated and experimental value of fraction of agglomerated metal for various compositions of HCS (see the section 3). It was established that at $k = 0.25$ the calculated and experimental data converge in the best way. Thus the coefficient k plays a role of matching coefficient.

Let's consider additional circumstances that were used for formalization of "pocket" and IPB concept. Firstly each basic particle must belong to two IPBs at least. Secondly each basic particle must form both the "pockets" and IPBs. Besides the minimum ratio between numbers of "pockets" and IPBs was introduced which is equal to 3. It should be noted that this value does not correspond to reality since a "pocket" can be identified repeatedly. Such restrictions allow model to exclude the situations that contradict the used conception of "pockets" and IPBs. It is important when jammed or loose packs are considered.

Described above principles are put in base of the model of microstructure of HCS. Input parameters of the model are the size distribution law of oxidizer particles and composition parameters of HCS (fractions and densities of components). The model can handle various size distribution laws and fractions number of oxidizer particles. The model allows determining the following characteristics:

- Density distribution function of sizes of "pockets" and mass-medium diameter of "pockets";
- Mass fraction of "pockets" in composition of HCS;
- Sizes of oxidizer particles that form the "pockets" of a certain size.

The developed model can be used for determining of parameters of microstructure of various HCS when the oxidizer particles form either jammed or loose packs and shape of particles is close to spherical. Let's consider the usage of the model for agglomeration process description.

3. Modeling results

Usage of the "pockets" and IPBs conception is very productive idea for agglomeration process description. Experimental results for various HCS [18 – 20] led to make a conclusion that only some part of initial metal is involved in agglomeration process. The conclusion is applicable for such types of HCS at burning of those the individuality of oxidizer particles is kept (not for ammonium nitrate-based HCS). Remainder part of initial metal burns out with formation of smoke oxide particles, i.e. not used to form agglomerates. The typical sizes of smoke oxide particles are $\sim 0.2 - 1.0$ μm [18 – 20]. These reasons caused introducing of concept of IPB as a part of composition that does not produce the agglomerates. The fraction of initial metal that form agglomerates Z_m^a depends on ratio between fractions of "pockets" and IPBs in initial HCS.

This circumstance is physically explained. It was established [18 – 20] that possibility of the agglomeration process realization is connected with formation of *skeleton layer* (SL). SL is a gas-permeable three-dimensional structure consisting mainly of the metal and its oxide as well as thermo-stable carbonic elements, and comprising the top portion of surface layer. For the most types of HCS the presence of "pockets" determines the possibility of the SL formation and thus realization of agglomeration process.

Depending on relation between carbonic layer decomposition temperature and metal fuel ignition temperature the SL can be classified as **A** or **B**-class. The temperature of metal fuel ignition is lower than the temperature of carbonic layer decomposition for the class **A**. Conversely it is higher for SL of class **B**. The ignition of metal leads to aluminum oxide melting inside SL and provide of liquid particles moving and merging [18 – 21].

The "pocket", "inter-pocket" and "pre-pocket" mechanisms of agglomeration were introduced [18, 19 etc.] which obviously affect on agglomerates sizes. At realization of "pocket" mechanism each agglomerate is formed by one "pocket". If "inter-pocket" mechanism is realized then each agglomerate is formed by several "pockets". On the contrary several agglomerates are produced from one "pocket" at "pre-pocket" mechanism realization. The presence of one or another mechanism depends on HCS type and chamber pressure.

The agglomerating particles evolution on the surface of burning HCS should be taken into account [21]. This process leads to change of physical chemical properties of agglomerate. In particular some part of metal in agglomerating particle burns out in gas-phase mode with formation of smoke oxide. That results in decreasing of parameter Z_m^a.

The physical picture description of formation of condensed combustion products as well as agglomeration process at burning of various types of HCS besides the papers [18 – 21] is also presented in [22].

The above circumstances give the possibility using model of microstructure to estimate important parameter of agglomeration process – a fraction of initial metal fuel participating in agglomeration (parameter Z_m^a). Besides, presence of the distribution function of "pocket" sizes provides possibility of modeling of the size distribution function of agglomerates (the mass size distribution density function $f_m(D)$) that are formed by the "pocket" mechanism of agglomeration. The question of effective usage of the model for determining of these parameters appears to be significant. The modeling results were compared with experimental data for various types of HCS.

Displays of influence of microstructure of HCS on agglomeration process are very various. Depending on properties of surface layer and agglomeration process character the four groups of HCS were distinguished:

I. HCS based on micron-sized Al, inert binder and various oxidizers. The properties of SL correspond to type **B** [19, 23];
II. HCS based on micron-sized Al, active binder [24];
III. HCS based on micron-sized Al, inert binder and mixture of oxidizer and ammonium nitrate [25];
IV. HCS based on micron or nano-sized Al, inert binder and various oxidizers. The properties of SL correspond to type **A** [19, 23];

The compositions of considered HCS are presented in referenced papers. The modeling results and their comparison with experimental data for listed types of HCS are presented below.

3.1 HCS of the First Group

In the low pressure domain (below ~ 0.5 – 1.0 MPa) as a rule the “pocket” mechanism of agglomeration is prevalent for these HCS. In the high pressure domain the influence of the “inter-” and(or) “pre-pocket” mechanisms increases [18 – 20]. Modeling results and their comparision with experimental data at P = 1.0 MPa [19, 23] are presented in Table 1.

Table 1: Modeling results for HCS of the **I** group

	I-1	**I-2**	**I-3**	**I-4**	**I-5**
D_{43}^{ox}, μm	25	152	237	500	175
D_{43}^{p}, μm	22	123	171	320	89
D_{43}^{a}, μm (calc.)	16	91	126	236	64
D_{43}^{a}, μm (exper.)	68 ± 10	98 ± 15	141 ± 20	504 ± 25	149 ± 15
Z_p	0.17	0.44	0.51	0.57	0.50
Z_m^a (exper.)	0.23 ± 0.02	0.35 ± 0.02	0.41 ± 0.02	0.45 ± 0.03	0.404 ± 0.04

On the Figure 4 the calculated mass size distribution density functions of agglomerates that are formed by “pocket” mechanism of agglomeration. On the Figure 5 the comparison of two of them with experimental data is presented.

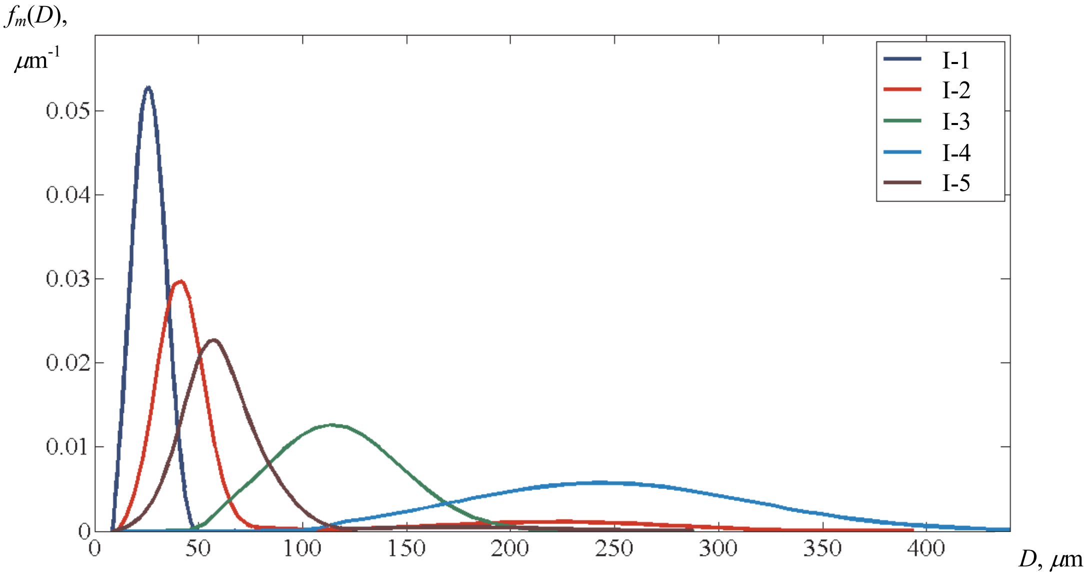
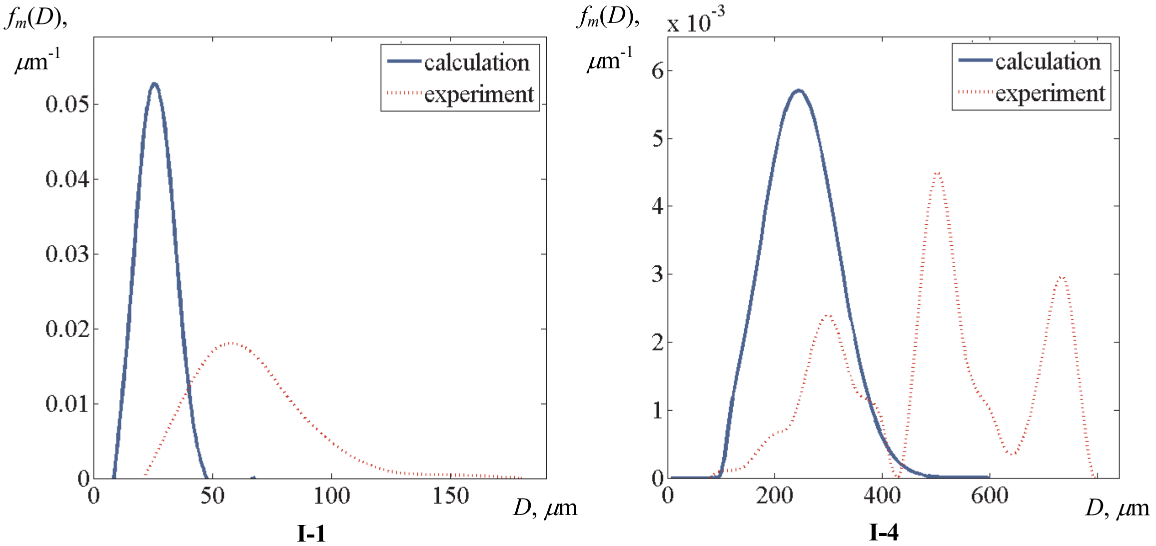


Figure 4: Calculated mass size distribution density functions of agglomerates for HCS of the **I** group (the “pocket” mechanism of agglomeration)



I-1 **I-4**

Figure 5: Comparison of calculation and experimental mass size distribution density functions of agglomerates for I-1 and I-4

Significant disagreement between calculated and experimental agglomerates sizes can be observed from Table 1 for several HCS (I-1, I-4, I-5). For I-4 it can be explained by "inter-pocket" mechanism presence at this pressure. It is confirmed by formations of modes in large sizes domain on experimental mass size distribution density function (Figure 5). For I-1 and I-5 an additional research must be performed for explaining of the mismatch.

It should be recognized that parameter Z_p can be used for estimation of mass fraction of initial metal that forms agglomerates. Some exceeding of parameter Z_p over Z_m^a is a consequence of combustion of a part of metal during evolution on the burning surface. The estimations of influence of evolution can be done [21]. A part about 25% of metal is burned out during evolution (Figure 6).

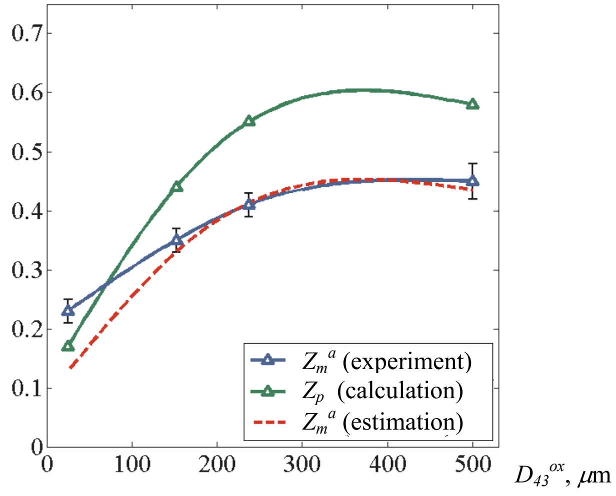


Figure 6: Comparison of calculation and experimental mass fraction of initial metal that forms agglomerates for I-1 – I-4

As it can be seen from Figure 6 the estimated and experimental values of Z_m^a converge well except of I-1.

3.2 HCS of the Second Group

The main feature of HCS of such group is reduced content of dispersed oxidizer relative to binder. Thus the microstructure has the properties of loose pack. Another feature is realization of agglomeration process in the low pressure domain only [24].

Results of the modeling are presented in the Table 2. The comparison of them with experimental data was performed for the parameter Z_m^a at $P = 0.8$ MPa.

Table 2: Modeling results for HCS of the **II** group

	II-1	**II-2**	**II-3**	**II-4**
D_{43}^{ox}, μm	83	70	108	77
D_{43}^{p}, μm	213	491	112	250
D_{43}^{a}, μm (calc.)	144	348	78.4	172
Z_p	0.48	0.54	0.39	0.52
Z_m^a (exper.)	0.45 ± 8 %	0.47 ± 6.7 %	0.33 ± 12 %	0.45 ± 5.5 %

Obviously the earlier conclusions on the possibility of using of the model for the agglomerated fraction of metal (Z_m^a) estimation are valid for HCS of the **II** group.

Results of estimation of D_{43}^a are valid only if the “pocket” mechanism of agglomeration is realized. It was established in paper [24] that the “pre-pocket” mechanism of agglomeration is prevalent in such conditions. So the direct comparison of calculated and experimental size distribution parameters of agglomerates and pockets cannot be made.

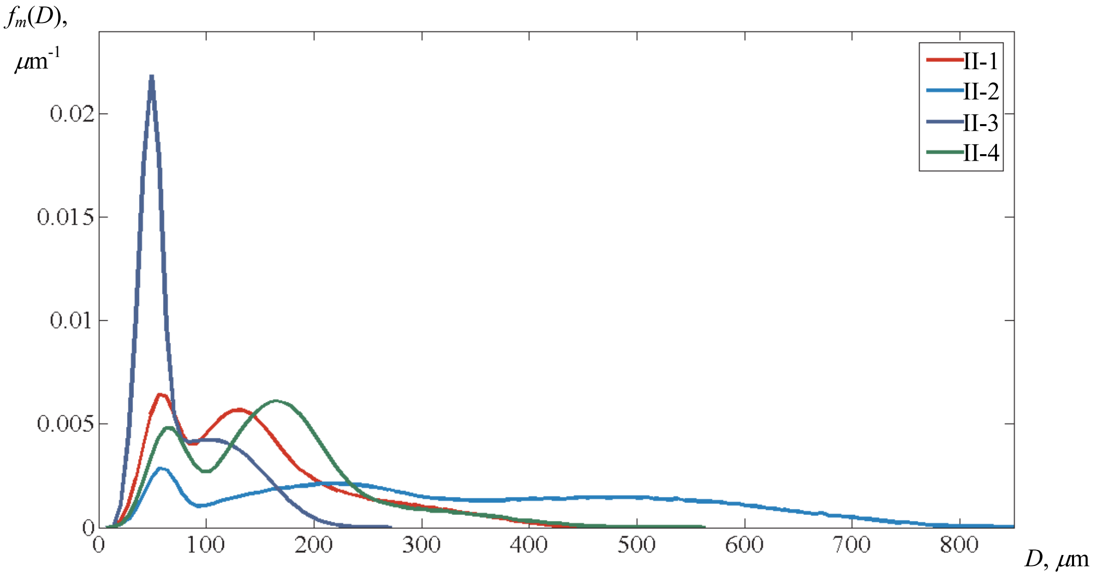


Figure 7: Calculated mass size distribution density functions of agglomerates for HCS of the **II** group (the “pocket” mechanism of agglomeration)

On the Figure 8 the results of estimation of influence of agglomerating particles evolution is presented. As it can be seen the exceeding of parameter Z_p over Z_m^a is ~ 10%. With this amendment the results converge quite well.

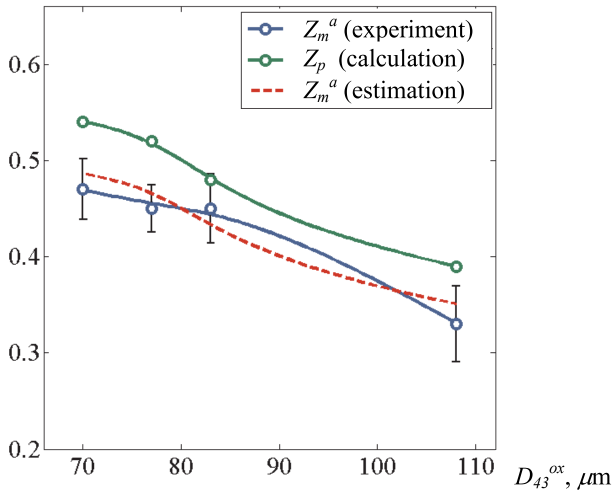


Figure 8: Comparison of calculated and experimental mass fraction of initial metal that forms agglomerates for II-1 – II-4

3.3 HCS of the Third Group

Modeling of microstructure of two HCS based on mixture of oxidizer and phase-stabilized *ammonium nitrate* (AN) was carried out. Results of the modeling are presented in Table 3. The experimental results were obtained for the high pressure domain at $P = 6.0$ MPa [25]. It should be noted that the different methods of phase stabilization of AN were implemented for III-1 and III-2 [25].

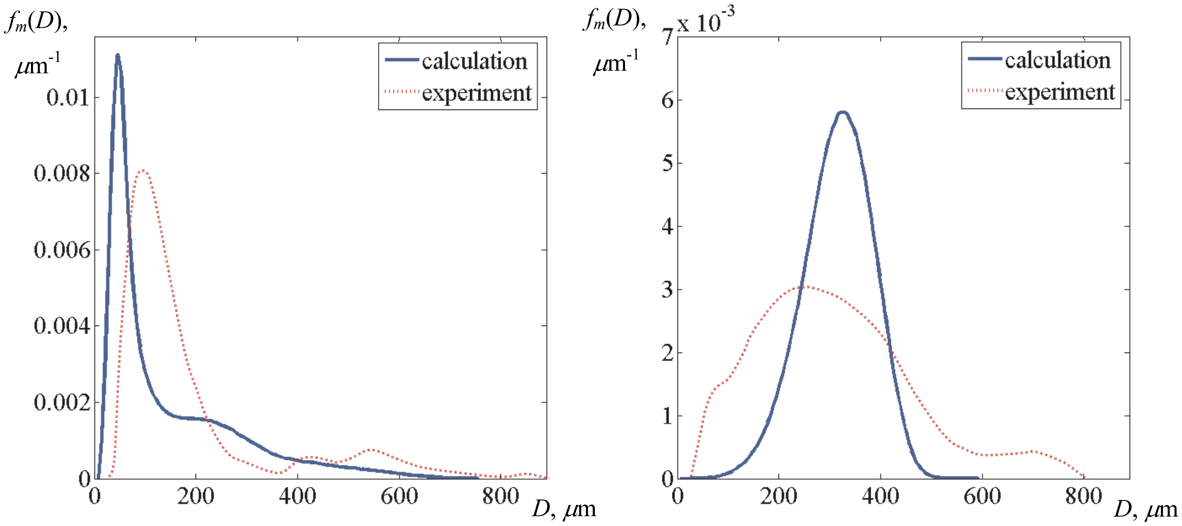
Table 3: Modeling results for HCS of the **III** group

	III-1	**III-2**
D_{43}^{ox}, μm	160	237
D_{43}^{p}, μm	251	532
D_{43}^{a}, μm (calc.)	190	303
D_{43}^{a}, μm (exper.)	184 ± 11.36	396 ± 52.34
Z_p	0.53	0.85
Z_m^a (exper.)	0.51 ± 9.12%	0.71 ± 8.34%

The agglomerates are formed mainly by the “pocket” agglomeration mechanism. However for the III-2 the inter-“pocket” merging occurs. In other words the regularities of burning of HCS based on pure AN appear increasingly [27].

On the Figure 9 the calculated functions of mass size distribution density of agglomerates and their comparison with experimental data from [25] are presented. For the III-1 formation of pockets is carried out by all oxidizer particles. But for III-2 the AN particles are not used to form structural formations. This distinction is the consequence of different methods of AN stabilization used in III-1 and III-2. At burning of III-2 the AN continuous melted layer is formed at the bottom part of SL. In other words the phase-stabilized AN particles in III-2 lose their individuality during combustion [25] like the pure AN-oxidizer particles [27]. The above feature of III-2 as well as AN-based HCS leads to significantly increasing of mass fraction of initial metal that forms agglomerates.

This circumstance is taken into account at modeling of the microstructure of III-2. The AN particles should be not used to form the structural formations in HCS. Nevertheless their presence affects on all oxidizer particles placing that is taken into account at determination of the used Poisson distribution law parameter.



III-1 **III-2**

Figure 9: Comparison of calculated and experimental mass size distribution density functions of agglomerates for HCS of the **III** group (the "pocket" mechanism of agglomeration)

Comparison of calculated and experimental data allows concluding that the model rather successfully solves the problem of estimation of agglomerating process parameters if the agglomerates are formed by the "pocket" mechanism.

3.4 HCS of the Fourth Group

HCS of the **IV** group are characterized by formation of SL only within the pockets like HCS of the **I** group. Unlike HCS of the **I** group a realization of the "pocket" mechanism appears in high pressure domain. At low pressures the "inter-pocket" and "pocket" agglomeration mechanisms take place [20]. At use of nano-Al these considerations are only valid if the metal particles keep their individuality in initial HCS [26].

The modeling results and experimental data from [23, 26] at P = 6.0 MPa are presented in Table 5. On the Figure 6 a comparison of calculated and experimental mass size distribution density functions of agglomerates.

Table 4: Modeling results for HCS of the **IV** group

	IV-1	**IV-2**
D_{43}^{ox}, μm	185	237
D_{43}^{p}, μm	112	138
D_{43}^{a}, μm (calc.)	82	97
D_{43}^{a}, μm (exper.)	101 ± 16	124 ± 18
Z_p	0.53	0.50
Z_m^a (exper.)	0.45 ± 0.042	0.48 ± 0.051

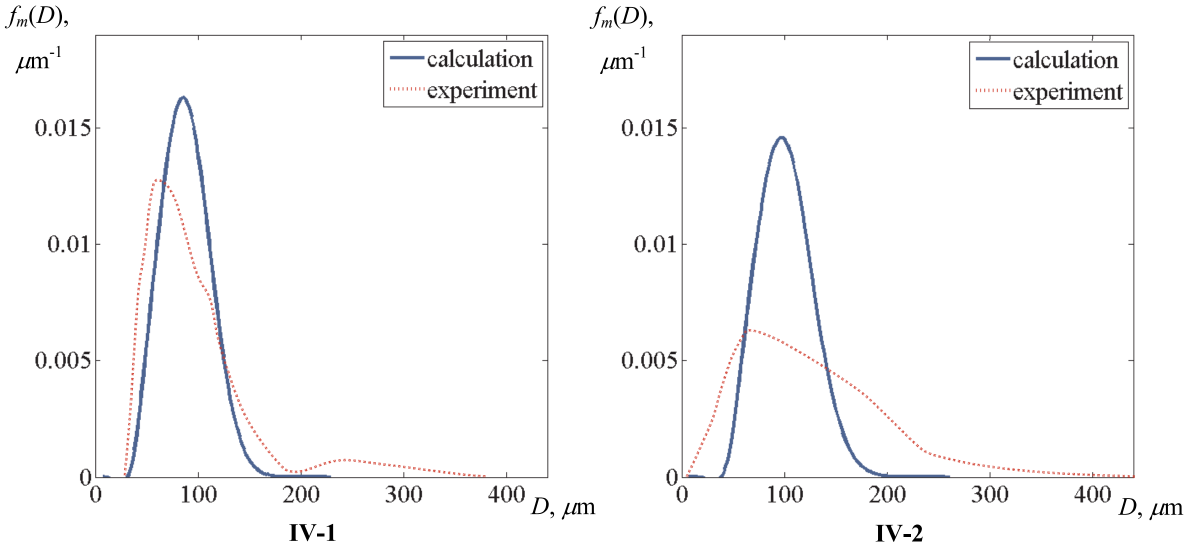


Figure 10: Comparison of calculated and experimental mass size distribution density functions of agglomerates for HCS of the **IV** group (the “pocket” mechanism of agglomeration)

The earlier made conclusions for efficiency of the microstructure model are applicable in case of HCS of the present group.

4. Summary and Discussion

Analysis of obtained results led to make a conclusion that generally the developed model of HCS microstructure solves the problem of *estimation* of agglomeration process characteristics. Some problems with correct using of the model appear in case of fine oxidizer presence in composition of HCS. Additional researches must be performed for understanding of the nature of these problems and their solving. In particular the question of assigning of D_{ox}^{min} value (the minimum size of oxidizer particles that form the pockets) still remains opened. The parametric analysis of the model displayed a significant influence of this parameter on the output data. Currently this parameter is used as matching coefficient. The used value of D_{ox}^{min} was equal 30 μm for HCS of the **II** group and 10 μm for other HCS.

Some discrepancy between calculated and experimental size of agglomerates for most of HCS can be explained by the presence of some amount of oxide in agglomerates. Moreover the shape of agglomerates differs from simple spherical drop. These circumstances can be taken into account at using of the model jointly with other descriptions of agglomeration process such as evolution of agglomerating particles.

It should be noted that modeling results depend significantly on accuracy of used distribution function of oxidizer particles sizes. So the fullness input data should be provided for correct usage of the model.

Parametric analysis of the model allowed to distinguish the factors that influence on characteristics of pockets. The most important factor is the size of oxidizer particles. Increasing of them leads to increasing of the sizes of “pockets” and increasing of their fraction in HCS. Presence of several oxidizer fractions that differ from each other by the size leads to formation of polymodal distribution of pockets.

Another significant factor is the fraction of oxidizer particles in composition of HCS. Increasing of them leads to decreasing of “pocket” sizes and their fraction in HCS.

The situations are possible at which smaller pockets appear within the larger pockets as well as within IPBs. This circumstance is supposed to lead to inaccuracy at microstructure parameters determination. However results of the analysis evidence that this inaccuracy is not significant.

It should be emphasized that proposed model provide solution of unique problem – predicting of the fraction of metal fuel that is involved in agglomeration process. It is shown that the problem can be solved by analysis of initial microstructure of HCS.

5. Conclusion

As a result of the work the following results were obtained:

1. The mathematical model of the microstructure of HCS was developed. The model allow determining the size distribution function of pockets and their fraction in HCS;
2. The analysis of modeling results for a various types of HCS was carried out. The modeling results were compared with results of experimental researches of agglomeration process;
3. It was shown that the model can be used for estimation of agglomerates size distribution density function as well as mass fraction of agglomerated metal relative to initial metal in HCS;
4. An influence on the microstructure parameters of various input parameters such as oxidizer size distribution function and oxidizer content is shown.

In general the obtained results allow considering of that model as one of the instruments for definition of characteristics of the condensed combustion products.

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