The Knowledge Base for Definition of Characteristics of the Condensed Combustion Products

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Abstract

Working out of means for creation of system of decision-making on properties of the condensed combustion products at a surface of burning composite condensed system is carried out. This system is based on ideology of expert systems. The developed means include knowledge base information support, and also decision-making principles. It is shown that properties condensed combustion products are defined by displays of process of burning: formation or not a skeleton layer, retention of individuality of oxidizer particles in a surface layer, difference between temperatures of ignition of metal fuel and decomposition of carbonaceous elements. Composition factors and the conditions of burning influencing these phenomena, and, hence, and on characteristics condensed combustion products are defined. The algorithm of an estimation of these characteristics is developed.

1. Introduction

Metal additives (as a rule, aluminum) are an indispensable component of *heterogeneous condensed systems* (HCS). A consequence of usage of this component is formation the *condensed combustion products* (CCP). Properties of these products make essential impact on quality of HCS. They define intensity of slag-formation in the chamber, intensity of interaction of combustion products with motor elements, and also level of losses of a specific impulse.

Formation CCP is carried out directly at a surface of burning HCS. Evolution of these products as a part of a flow of combustion products takes place further. It is possible to assert that the HCS burning makes essential impact on properties CCP and quality of HCS is defined, including, and characteristics of these products.

Despite numerous attempts of mathematical modeling of formation process of the condensed products at a surface of burning HCS, the problem of forecasting of CCP properties depending on parameters of HCS composition and burning conditions is not solved by this time [1]. The situation is in many respects similar to a situation with modeling of burning process and forecasting of the law of burning rate: numerous works are performed on modeling of burning process; however the results used for practical purposes obtain only at carrying out of experimental works.

Told above has allowed to draw a conclusion on expediency of use of approaches of the theory of expert systems for definition (estimation) of CCP characteristics.

The purpose of the present work was development of components of this system and, first of all, knowledge base information support. The carried out work is based basically on the results obtained in Baltic State Technical University.

The condensed products leave a surface of burning HCS as a part of two fractions: agglomerates and smock oxide particles (SOP). Obtaining of the following information for description CCP is expedient.

1. Fraction of initial metal in HCS used to form agglomerates (Z_m^a). This parameter defines involvement degree metal fuel in agglomeration process.
2. Mass function of size distribution density of agglomerates ($f_m(D)$ and mass function of size distribution density of smoke oxide particles ($f_m(d)$).
3. Mass fraction of oxide in agglomerate (η).
4. Type of agglomerates. (Four types of agglomerates are known now: “matrix” agglomerates; agglomerates with “cap” oxide; “hollow” agglomerates; agglomerates with continuous oxide layer.)

2. The general physical picture of formation CCP

The analysis of an experimental material available by this time [2-12] has allowed formulating the general representations about the physical nature of processes of formation CCP at a surface of burning HCS. All set of the condensed products is divided traditionally on two basic fractions: agglomerates and smock oxide particles.

Agglomerates are products of integration of the condensed products in a surface layer of HCS. Smock oxide particles are products of combustion of not agglomerating metal in a zone of a gas phase over a surface of burning HCS, and also combustion of agglomerating metal in gas-phase mode in a surface layer of HCS. Properties of a surface layer play a key role in processes of formation of these particles. These properties are defined by characteristics of a skeleton layer (SL). The skeleton layer is a gas-permeable three-dimensional structure consisting mainly of the metal and its oxide, as well as thermostable carbonic elements, and comprising the top portion of surface layer (fig.1). The specified structure arises, as a rule, at HCS burning. It provides coherence of particles of initial metal and possibility of a delay of agglomerating particles in a surface layer, i.e. possibility of *realization of agglomeration process*. It is shown that a necessary condition of SL formation is formation of a carbonaceous skeleton (CS). Formation of this structure, in turn, is connected with conditions of decomposition of the polymeric binder.

Completeness of transformations at decomposition increases, i.e. the probability of formation CS falls, if concentration of oxidizing substances in the field of decomposition increases. These substances can contain as in binder (active binder), and to appear owing to diffusion from area of particles decomposition of coarse fraction of an oxidizer. Thus, it is possible to specify the factors promoting disappearance at burning CS, and, hence, and a skeleton layer: presence active binder or pseudo-active binder (presence in binder fine oxidizer fractions), and also decomposition of narrow layers of binder between large oxidizer particles.

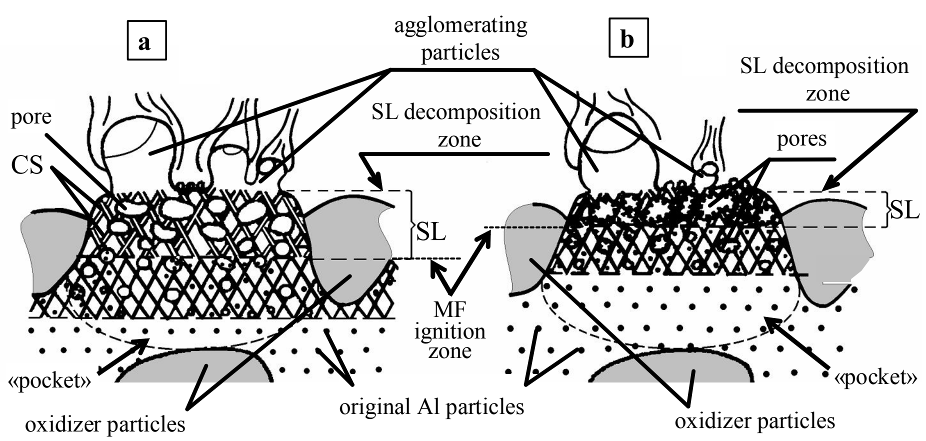


Figure 1: Sketch of skeleton layer in burning of HCS of a) class **A** and b) class **B** [3]

Such concept as "inter-pocket bridge" – binder layers between oxidizer particles in which limits SL it is not formed has been entered [2-3]. If oxidizer particles in surface layer lose the individuality, for example, owing to rather early fusion the specified layers cease to correspond "inter-pocket bridges".

Absence SL leads to that combustion of initial metal fuel in a zone of a gas phase over a surface of burning HCS takes place. Duration of a stage of heterogeneous burning is longer owing to rather low ignition temperature in this situation. It leads to that the role of this burning mode increases in formation SOP [9]. A formation smock oxide particle in the presence of SL is connected with combustion of agglomerating particles on the top surface skeleton layer in gas-phase mode [9].

Properties SL define properties of the formed condensed products. These properties depend on character of behavior of metal fuel and carbonaceous elements in a surface layer. Two classes' HCS depending on difference between temperature of metal ignition (T_{igm}) and temperature of decomposition of carbonaceous elements (T_{dc}) have been entered: **A** and **B** [3]. Condition $T_{\mathrm{igm}} < T_{\mathrm{dc}}$ is for HCS class **A**, and for HCS class **B** – $T_{\mathrm{igm}} > T_{\mathrm{dc}}$. For HCS class **A**, the top part SL is the carbonaceous skeleton, which pores is filled liquid by metal and it oxide. For HCS class **B**, the top part KC is the metal skeleton consisting of initial particles of metal. It is obvious that properties of agglomerates at burning топлив the specified classes are various. For HCS class **A**, the fraction of the metal, which is burning down in a heterogeneous mode, increases that conducts to content increase oxide in agglomerates. Besides, level of the adhesive forces keeping agglomerating particles on top surface SL increases, a consequence of that, as a rule, growth of the size of agglomerates is.

Thus, properties CCP depend on displays of burning process the cores among which are:

- formation or not a skeleton layer;
- conservation or not individualities of oxidizer particles (OXP) in a surface layer of HCS;
- difference in the conditions of ignition of metal particles and decomposition of carbonaceous elements.

The decision of a question on character of realization of these phenomena has basic value for an estimation of properties CCP (fig. 2).

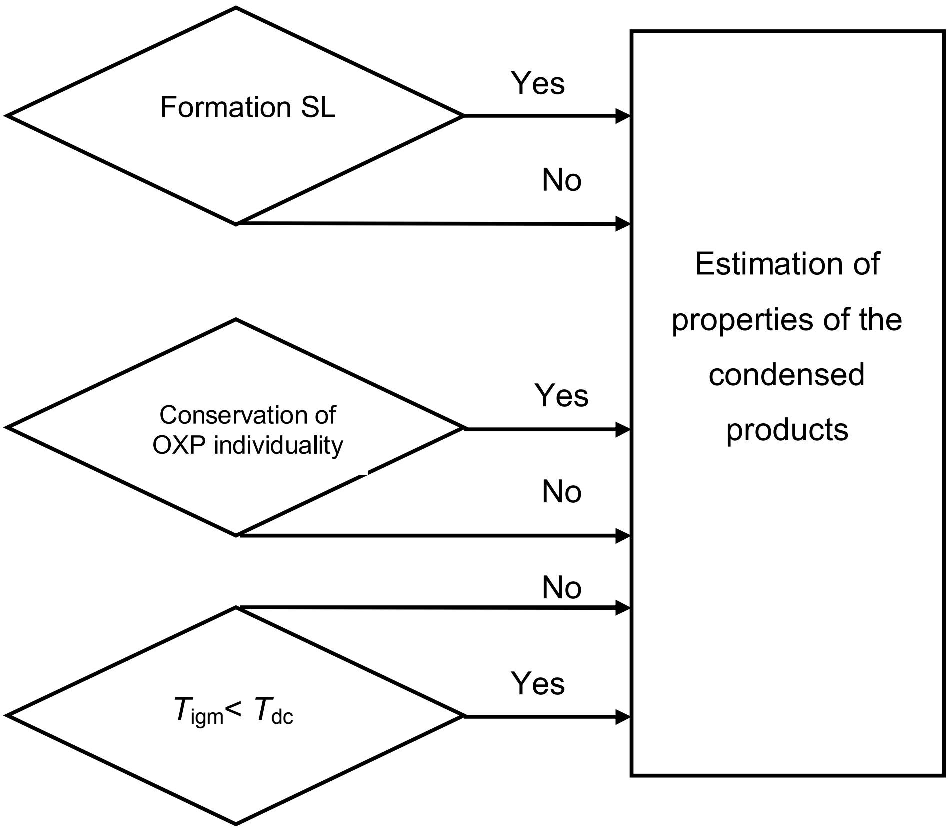


Figure 2: The scheme of an estimation of condensed products properties

Let's consider influence of parameters of HCS composition on properties of surface layer, i.e. on specified above the phenomenon, and, hence, and on CCP properties at a surface of burning HCS.

3. Parameters of HCS composition and CCP properties

Properties CCP are defined by characteristics of surface layer of burning HCS which define laws of processes as agglomerations, and formations smock oxide particles. Considering this circumstance, pertinently to use results of work [4] in which depending on composition parameters allocation of types HCS with close laws of formation of a surface layer is carried out.

Following types HCS are allocated.

1. HCS on the basis of inactive binder, micro-sized aluminum and oxidizers of a various kind.
2. HCS on the basis of active binder, micro-sized aluminum and oxidizers of a various kind.

3. HCS on the basis of inactive binder, micro-sized aluminum, mixture of oxidizer and ammonium nitrate
4. HCS on the basis of inactive binder, nano-sized aluminum and oxidizers of a various kind.

3.1 HCS of the first type

Presence inactive binding and oxidizers, which keep the individuality, leads to that formation of a skeleton layer, and, hence, and agglomerates occurs only within "pockets" and does not occur in "inter-pocket bridges". The mass fraction of "pockets" in HCS makes defining impact on a share of the metal fuel forming agglomerates – Z_m^a (fig. 3).

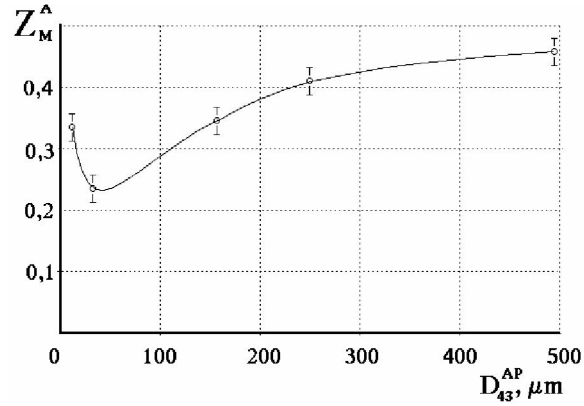


Figure: 3 Dependence of parameter Z_m^a on the size of oxidizer particles [2]

Properties of a skeleton layer correspond HCS a class **B**. The size of agglomerates is defined by possibility of realization of three mechanisms of agglomeration: "pre-pocket", "pocket" and "inter-pocket" [3]. The basic type of agglomerates for these HCS is agglomerate with "cap" oxide [5] (fig. 4). Agglomerates consist of metal and oxide. The mass fraction value of oxide (η) is in an interval 0.1-0.35.

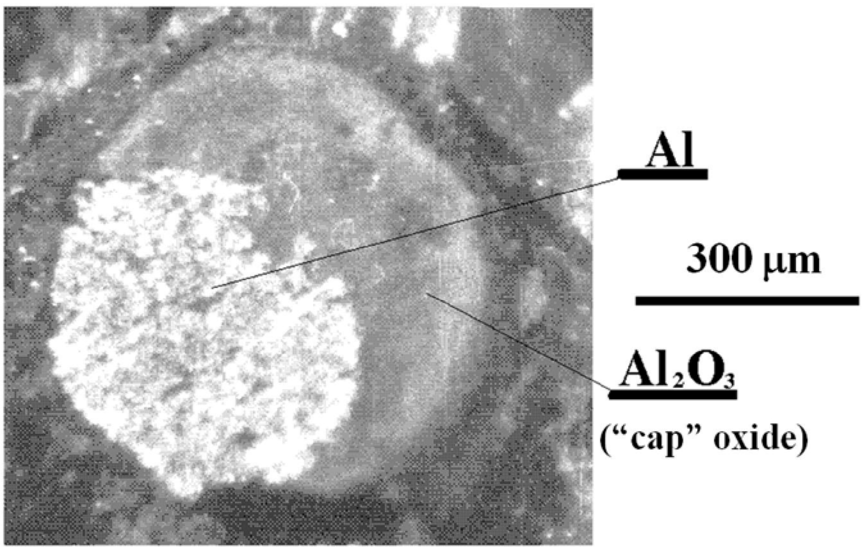


Figure 4: Microsection of the agglomerate

Formation SOP (fig. 5) it is carried out owing to combustion of not agglomerating metal fuel and burning of metal of agglomerating particles on the top surface SL in gas-phase mode [9]. Mass-average diameter of smoke oxide particles at low intensity of agglomeration process is in narrow enough range of 350-450 nm, and at high - in wider range of 450-800 nm. Mass function of size distribution density of smoke oxide particles generally is two-modal. The quantity of the particles forming a mode in the domain of the big sizes is prevailing (fig. 6).

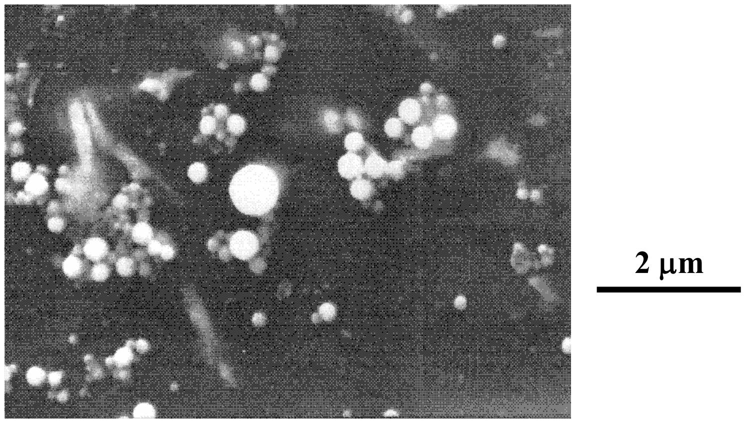


Figure 5: Smoke oxide particles quench-collected at the burning surface [3]

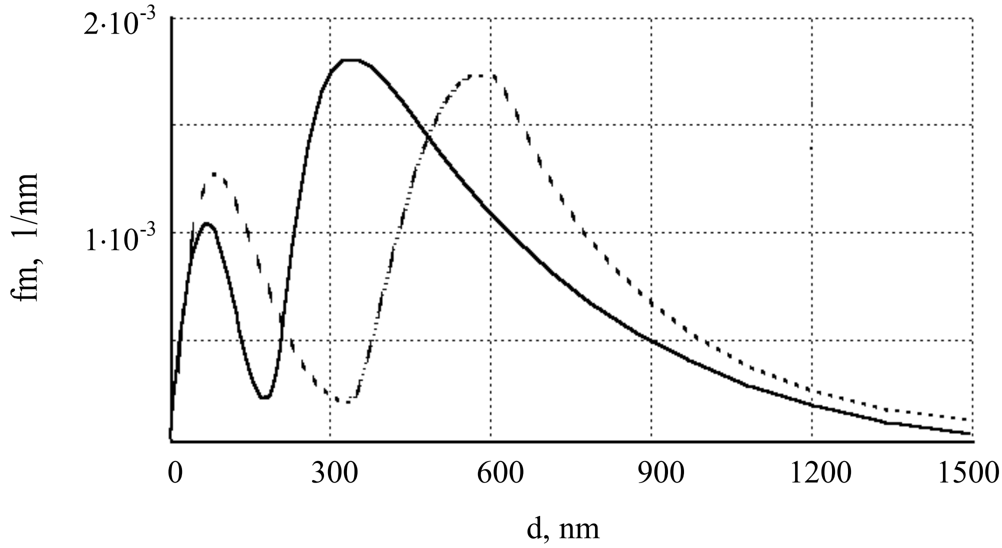


Figure 6: Functions f_m(d) for two HCS at 6.0 MPa [3]

3.2 HCS of the second type

Preconditions for absence of formation of a skeleton layer owing to presence of the active binder are for HCS this type. Laws of formation SL, and, hence, and agglomerates depend on pressure value. In the domain of low pressure, these laws are similar to corresponding laws HCS the first type, but SL practically disappears at transition in domain of high pressures that leads to sharp falling of a mass fraction of agglomerates in CCP composition [6].

The device providing delimitation of domains of high and low pressure for considered type HCS is absent now. However, apparently, pertinently to speak about domain of high pressures at pressure from above 5.0 МПа for all HCS this type. Parameter Z_m^a does not exceed value of 2-4 % in this domain that allows to exclude practically from consideration agglomerates (fig. 7).

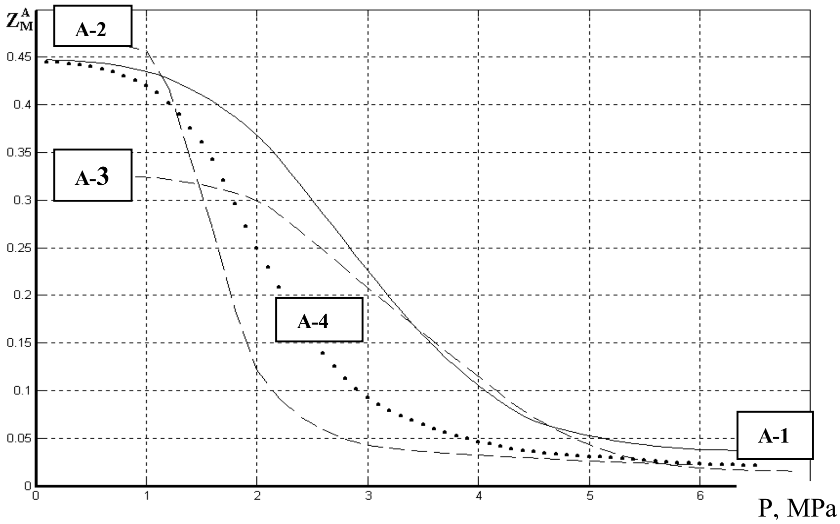


Figure 7: Dependences $Z_m{}^a$(P) for four HCS on the basis of the active binder (A-1 – A-4) [6]

The skeleton layer formed in the domain of low pressure on the properties corresponds HCS **B** class [6].

The mass- medium size of d_{43} makes 700-800 nanometers that on the average above in comparison with HCS the first type. Mass function of size distribution density of smoke oxide particles is close to unimodal (fig. 8).

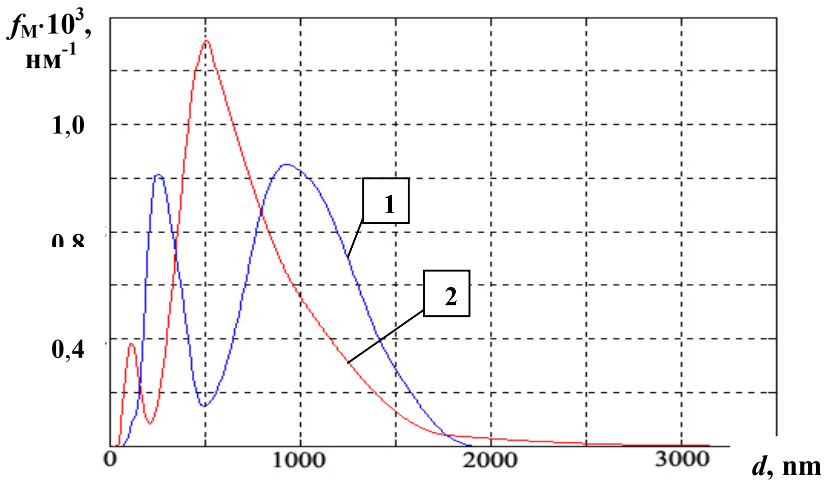


Figure 8: Functions f_m(d) for HCS the first (1) and second (2) type [9]

3.3 HCS of the third type

Fusion at rather low temperature is characteristic for ammonium nitrate (AN). This circumstance leads to that the fused oxidizer fills the bottom part of a surface layer and decomposition of the binder is carried out approximately in identical conditions. A consequence of it is that layers between oxidizer particles cease to carry out functions of "inter-pocket bridges", i.e. SL is formed in all structural formations of HCS [5].

Rather early ignition of metal fuel leads to that SL properties correspond HCS **A** class. It represents the carbonaceous skeleton which pores are filled by “liquid Al-Al_2O_3”. Distinctive feature is the considerable share of the metal which is burning down in a heterogeneous mode within SL. Besides, for these HCS long time of stay of agglomerating particles for the top surface SL (to hundreds ms) is characteristic that leads to increase of a role of process of evolution of these particles. The specified process includes metal burning in gas-phase mode, structure change, interaction of the condensed metal and oxide, feeding and merging of particles.

The specified properties of a surface layer [5] lead to following consequences:

- The fraction of the metal fuel forming agglomerates, reaches considerable values (Z_m^a ~80%).
- Agglomerates consist basically from oxide (η ~85%).
- The basic type of agglomerates is agglomerate with "cap" oxide.
- The size of agglomerates reaches considerable values. It can make sizes ~1000 microns (Fig. 9).
- Mass function of size distribution density of smoke oxide particles has unimodal character. The mass-medium size of these particles is in an interval of 700-1000 nanometers [9].

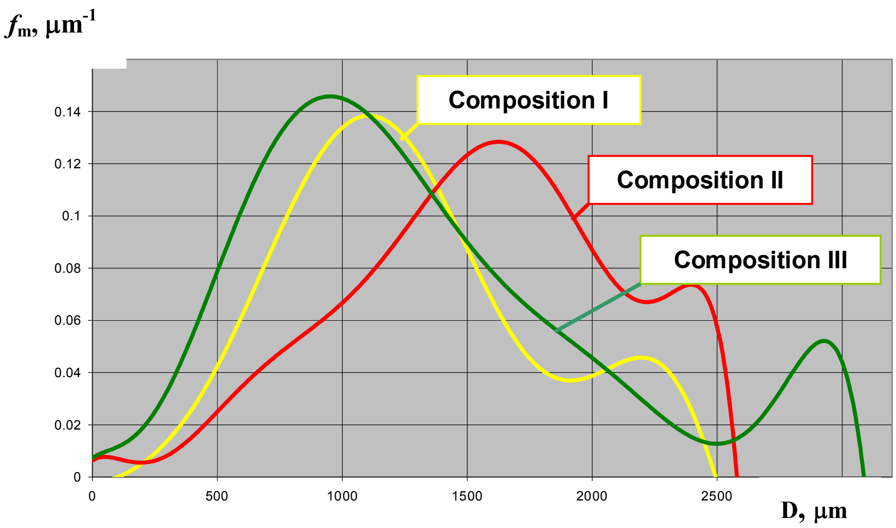


Figure 9: Functions f_m(D) for three AN-based HCS (I –III) at 6.0 MPa [5]

Phase stabilization AN can change behavior of this oxidizer in a surface layer [7]. If "the thermodynamic" method is used, oxidizer particles keep the individuality in a surface layer that leads to change of laws of formation SL, and, hence, and - the condensed products. Other methods do not change behavior AN in a surface layer, i.e. phase-stabilized AN as well as "pure" AN loses the individuality in a surface layer.

3.4 HCS of the fourth type

Laws of formation SL depend on, whether keep initial particles of metal in HCS the individuality or form the connected structures.

HCS of considered type it is possible to divide in turn according to realization of two specified above situations, using terminology of works [10, 12], on HCS of type Nano1 and Nano2.

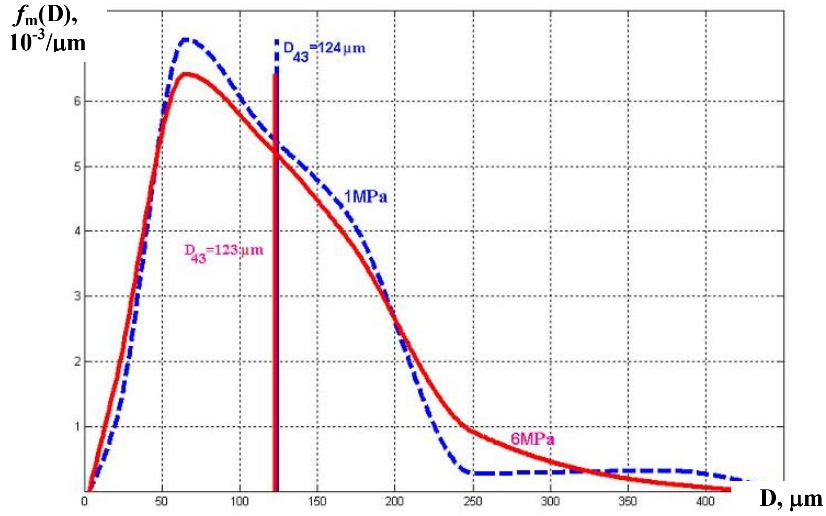
Properties of SL of HCS type Nano1 are similar to properties SL class **A** HCS.
If in HCS the oxidizers retention the individuality, the share of the metal fuel forming SL depends on quantity and the size of oxidizer particles. Thus, it is possible to speak about realization of laws of burning HCS the first type. Thus, the basic mechanisms are "pocket" and "inter-pocket", the type of agglomerates corresponds "matrix" and with "cap" oxide.

Properties SL HCS type Nano2 are close to properties SL class **B**. Formation SL is connected neither with HCS structure, nor with conditions of its burning. All it has allowed to draw a conclusion that properties similar SL are defined by manufacturing techniques. Experimental data testify to rather considerable fraction of metal participating in its formation. Parameter Z_m^a has high value (~0.9-0.95) which practically does not depend on pressure [10].

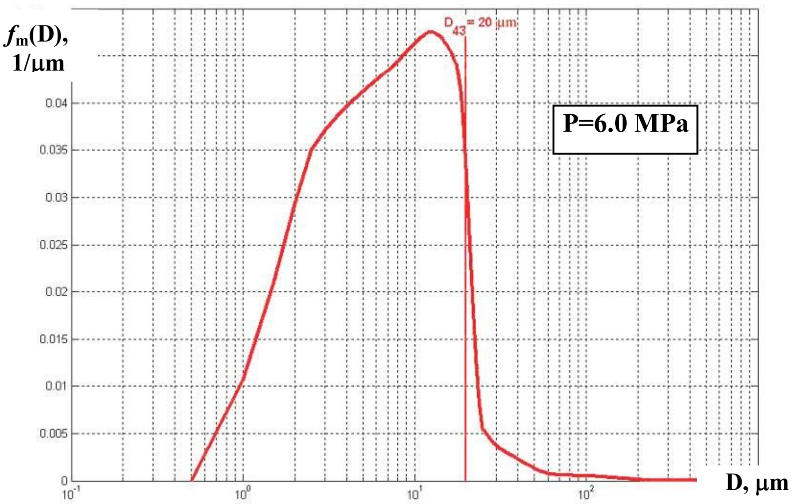
Features of agglomerates at burning HCS type Nano2 are:

- rather small sizes of agglomerates (~ several tens micron) (this size almost 10 times less the size of agglomerates for HCS type Nano1);
- possibility of formation of agglomerates which represent a metal particle covered with rather thick cover of oxide [10].

Functions $f_m(D)$ for HCS which concern types Nano1 and Nano2 illustrating essential difference at a size of agglomerates are resulted on fig. 10.



a)



b)

Figure 10: Functions $f_m(D)$ for HCS type Nano1 (a) and Nano2 (b) [10]

It is natural that the experimental material available now not to the full reflects character of influence of composition parameters and burning conditions on properties of the condensed products. It is possible to name variety of "white stains" in the description of CCP formation. It is possible to name among them, for example, the following: burning HCS on the basis of such perspective oxidizer as a hydrazinium nitroformate, burning at elevated pressures (from above 10.0 MPa) etc.

Besides, number uncertainties the various factors connected with influence on characteristics CCP exists within the limits of resulted above the description.

It is possible to name among them:

- borders of domains on pressure and the content of oxidizing elements in binder, in which limits the skeleton layer is not formed;
- ratio between the content micro-sized and nano-sized metal providing realization of mechanisms of burning HCS classes **A** and **B**;
- character of influence of type of an oxidizer on realization of mechanisms of burning HCS classes **A** and **B**;
- realization conditions «pre-pocket» and "inter-pocket" mechanisms of agglomeration.

4. Calculation means for definition of CCP characteristics

Calculation means are based on the analysis of the mathematical models describing those or other phenomena which are connected with formation of the condensed products. Quantity of the models allowing to obtain significant for practical purposes results it is rather insignificant [1].

Let's consider models which are based on the experimental material described above.

A. *Model of structure of HCS* [14-15]
For conditions when the oxidizer in a surface layer keeps individuality, the model provides definition of function of size distribution density of "pockets" in and shares of "pockets" and «inter-pocket bridges» in HCS. This information provides possibility of an estimation of the size of agglomerates and parameter Z_m^a.

B. *Model of agglomerates dispersion* [16]
The model provides for HCS a class A, in conditions when "pocket" and "inter-pocket" mechanisms of agglomeration are realized, definition of function of size distribution density of agglomerates.

C. *Model of evolution of agglomerating particles* [17]
The model describes physical and chemical transformations of agglomerating particles on the top surface SL and allows to define a chemical composition and parameters of agglomerates structure.

D. *Complex model of agglomeration* [17]
The model provides synthesis of models A, B, C and allows for HCS a class **A** (oxidizer particles keep the individuality) to define all properties of agglomerates: the size, share as a part of combustion products, chemical composition, structure.

Possibilities of the considered models are schematically shown on fig. 11.

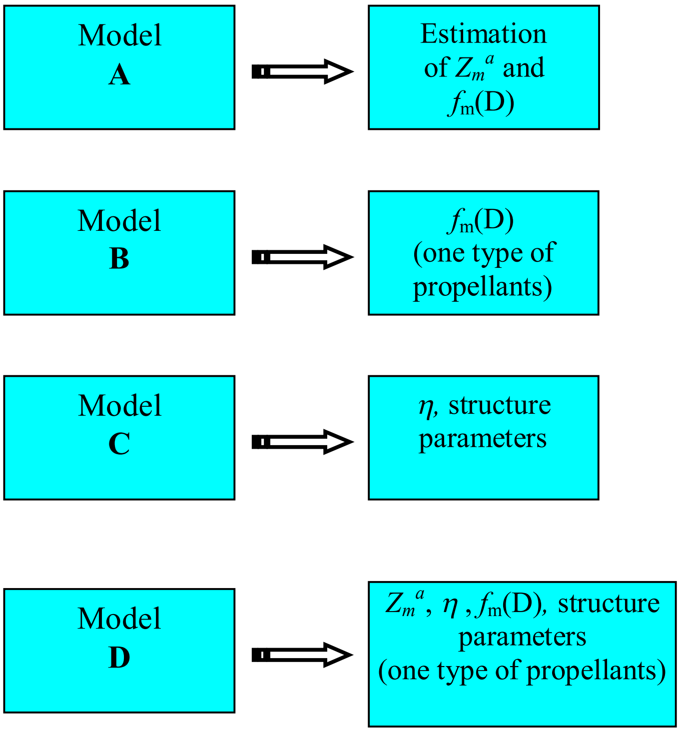


Figure 11: Possibilities of calculation means for definition of agglomerates characteristics

Let's underline that the means describing SOP dispersion at a surface of burning HCS are unknown to us.

5. Principles of system of decision-making on properties CCP

Obvious uncertainty of knowledge of laws of CCP formation does expedient at decision-making on properties КПС to use ideology of expert systems. The carried out analysis has shown that the decision-making system should be based on use of the device of indistinct sets and the indistinct logic [18].

The mathematical theory of indistinct sets and the indistinct logic are generalizations of the classical theory of sets and the classical formal logic. The indistinct logic allows to model processes, using high enough level of abstraction, and does not demand exact and unequivocal formulations of laws.

Introduction procedure membership function and actions with them for acceptance of any decision lies underlies the used device. The basis for drawing up of these functions (fuzzification procedure) and decision-making (defuzzification procedure) is experience of experts which authors of system are.

The created system is based on the algorithm which scheme is shown on fig. 12. Basic value has influence of those or other factors on displays of burning process which were discussed earlier (fig. 2). The decisions connected from realization of specified displays, are accepted according to a set of rules which are based on positions of indistinct logic.

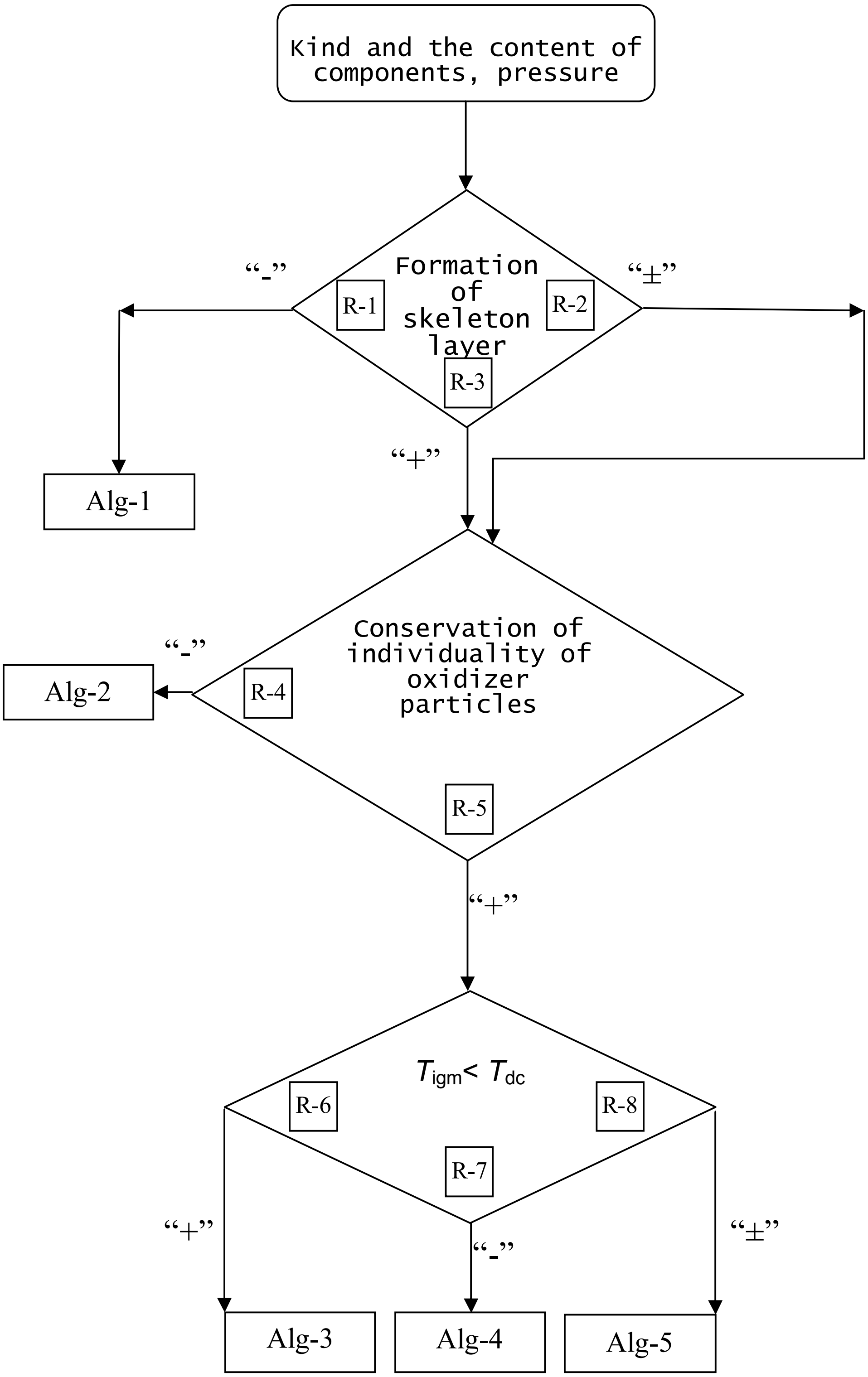


Figure 12: The scheme of decision-making on properties CCP ("-" – the condition is not carried out, "+" – the condition is carried out, "±" – the condition is carried out partially, R-1,..R-8 – rules, Alg-1,..Alg-5 – algorithms of an estimation of properties CCP)

Let's consider as an example use of rules of definition of possibility of formation SL depending on value of pressure and «activity degree» the binder.

Let's enter two linguistic variables: *pressure* and *type of the binder*. The variable "pressure" will include three terms: small, average, big. It is carried out fuzzification by this variable and membership function - $\mu(P)$ (fig. 13) is entered.

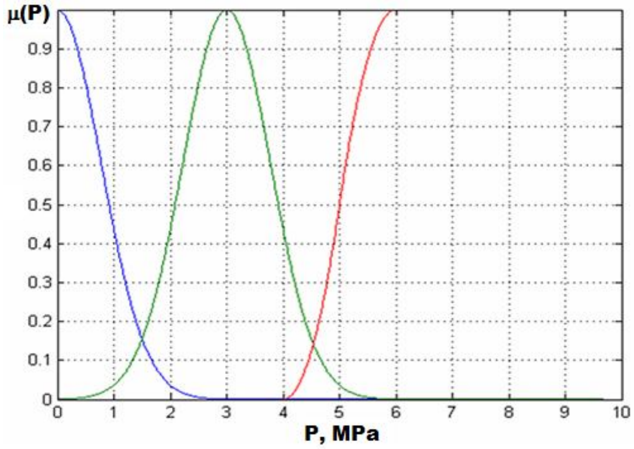


Figure 13: Function μ(P)

Variable «type binder» also we will break into three terms: inactive, small-active, active. Activity of the binding depends on an oxidizer mass fraction; therefore membership function of terms of this variable will be functions from the content of oxidizing elements as a part of binding - μ(O) (fig. 14).

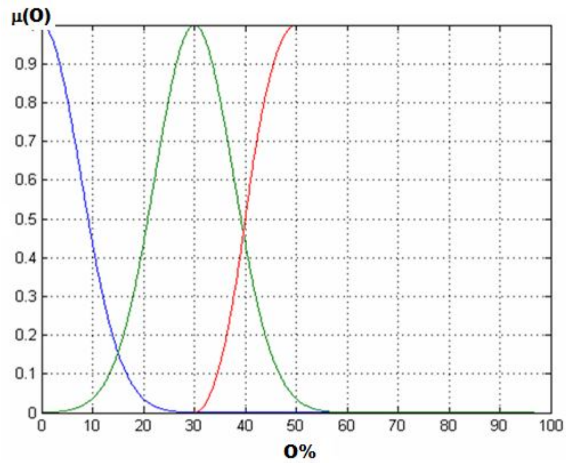


Figure 14: Function μ(O)

Let's formulate rules which define the various situations connected with SL formation:

1. If “pressure big” and “binding active” are, SL it is not formed.
2. If “pressure an average” and “binding active” or “pressure average” and “binder small-active” or “pressure big” and “binder small-active” are, SL it is partially formed.
3. If “pressure small” or “binding inactive” is, SL is formed.

At a decision choice, the rule is activated, which corresponds to the maximum value of membership function.

After decision-making on character of displays of process of the burning, the choice is carried out one of algorithms of an estimation of characteristics CCP (fig. 11). These algorithms assume use of computing procedures (at their presence) and the experimental data obtained for situations which are close to the considered. The obtained information is accompanied by the data about accuracy and comments which include characteristics of used means.

6. Conclusion

Following basic results are obtained at carrying out of the present work.

1. The basic phenomena defining the characteristics of condensed products at a surface of burning HCS are defined on the basis of the analysis of a physical picture of burning process.
2. The major composition factors of structure influencing characteristics CCP are established.
3. Calculation means for definition of characteristics CCP are analyzed.
4. Principles of system of decision-making on properties CCP are developed.

Results of work urged to become a basis for creation of the new approach to the description of such difficult process as process of burning of HCS.

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