5th European Conference for Aeronautics and Space Sciences
Munich, Germany, 1-5 July 2013

Model of Composite Solid Propellant Microstructure and Problem of Agglomeration Process Description

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There is no doubt that the microscopic structure inhomogeneities affect on the physical and mechanical properties of the composite propellants as well as on their burning process. Therefore a development of an adequate model of the microstructure of composite solid propellants is quite important. Structure description should be put in a base of agglomeration process description as well as the burning process description in the whole.

In the present paper we consider the method for the modeling of the composite propellants microstructure and usage of the modeling results for description of agglomeration – one of the phenomena of burning process.

By the present time various approaches for the modeling of the heterogeneous materials microstructure are existent that are based on concept of representative volume. The particles of dispersed phase are placed inside the representative volume. Various packing algorithms were implemented by several authors: T.L. Jackson et. al., F. Maggi et. al, S. Gallier, S.A. Rashkovskii and others. Based on such structure descriptions a few agglomeration numerical models were proposed.

In our opinion, not solved problems are available in the carried out works. It is absence of substantiation at a choice of the law of distribution of the particles centers in propellant volume and interpretation of results of modeling for the description of burning process.

In the present work the conception of “pockets” and “inter-pocket bridges” is used for the structure description. A “pocket” consists of metal fuel particles, fine oxidizer particles and binder and appears between several coarse oxidizer particles. An “inter-pocket bridge” is a part of “metal fuel – fine oxidizer – binder” composition that enclosed between two adjacent coarse oxidizer particles. According to this approach propellant microstructure can be represented by coarse oxidizer particles, “pockets” and “inter-pocket bridges”.

Let’s consider main principles of the model:

- The Monte Carlo method is used. The centers of particles are distributed within propellant volume under the law of Poisson. Correction of the distance between particles centers is performed if the particles overlap.
- A planetary model is used for description of local structure around “basic” particles. Results of the analysis of the surroundings of a large number of “basic” particles allow to tell about propellant characteristics as a whole.

- 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.
- A volume of “inter-pocket bridge” is determined using the coefficients obtained by means of comparison of calculated and experimental data.

Input parameters of the model are the size distribution law of oxidizer particles and propellant composition parameters (fractions and densities of components). The model can handle various size distribution laws and fractions number of oxidizer particles.

The main output data of the propellant microstructure model are the density distribution function of “pocket” sizes and mass fraction of “pockets” in propellant composition.

Displays of influence of propellant structure on agglomeration process are very various. The formation of skeleton layer for a number of types of propellants and, hence, and agglomerates occurs only within "pockets". This circumstance gives the possibility using model of propellant structure to define important parameter of agglomeration process – a fraction of the metal fuel participating in agglomeration. Besides, presence of the distribution function of “pocket” sizes provides possibility of modeling of the size, structure and a chemical composition of agglomerates.

The modeling results were compared with experimental data for propellants based of AP, ADN and AN-AP containing micron-sized as well as nano-sized aluminium and for propellants containing active binder (for the low pressure domain only). The main regularities are represented rather accurately that evidences on high quality of the model for the description of agglomeration process. It is not excluded that developed model can be used at describing other burning phenomena as well as physical and mechanical properties of composite propellants.