Modeling of Heterogeneous Structure and Properties of Composite Solid Propellants

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ABSTRACT

The problem of heterogeneous solid propellant modeling is addressed in different studies including evaluation of properties of energetic materials and combustion simulations. Practical composite propellants can contain several particulate components, characterized by a wide range of size distributions (from less than 1 μm to several hundreds of μm) and very different physical properties (compare for example AP, HMX, Al), which are fixed in a polymer binder. Because of purely random organization, such materials cannot be described in a general manner and require a specific modeling approach. In the present paper, we consider two important stages of solid propellant modeling: particle packing generation and heat transfer simulation based on the finite volume method.

In application to the solid propellant modeling, generation of a random particle packing is a complicated task because of a high required packing density, a wide particle size distribution, and a large number of particles. With these conditions, the computational efficiency of the packing method is of primary importance. From this point of view, we compare two different methods: the method of Lubachevsky-Stillinger (LS) and the random sequential adsorption (RSA). Both methods have been realized using several numerical techniques to minimize the computational cost of packing generation. Traditionally LS is considered as a computationally intensive method capable to produce dense packing whereas RSA is much cheaper but not suitable because of low packing density. Based on several examples of solid propellants we demonstrate that RSA can be successfully used resulting in sufficiently dense packings of the order of 10^5-10^6 particles.

To model the heat transfer in a heterogeneous material, one starts with discretization of a simulated sample, which consists in mapping of a particle packing onto a discrete computational mesh. In the present paper, we consider a structured Cartesian mesh, which is convenient for solving a coupled problem of solid propellant burning with nonuniform surface regression. At this stage, the mesh step imposes a certain level of numerical error, which must be properly handled. As an example, in a cubic domain of 1 mm size, a uniform mesh of 10^6 cells has a step of 10 μm hence particles of several tens of μm in diameter will be represented with significant errors and those, whose size is of the same order or less than the mesh step, will be fully altered by the discretization. In this situation, one must look for a numerical method with a low sensitivity to the numerical errors. We have applied the finite volume method, which provides progressive degradation of particle representation when the mesh step approaches the particle diameter and the conservation property of the numerical solution. Our numerical tests show that, with a proper choice of the mean conductivity formulation, the numerical error can be minimized.