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Using level sets for creating virtual random packs of non-spherical convex shapes

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ABSTRACT

Random packs of spheres have been used to model heterogeneous and porous material morphologies during simulations of physical processes such as burning of coal char, convective burning in porous explosives, and regression of solid rocket propellant. Sphere packs have also been used to predict thermo-mechanical properties, permeability, packing density, and dissolution characteristics of various materials. In this work, we have extended the Lubachevsky–Stillinger (LS) sphere packing algorithm to create polydisperse packs of non-spherical shapes for modeling heterogeneity in complex energetic materials such as HMX and pressed gun propellants. In the method, we represent the various particle shapes using level sets. The LS framework requires estimates of inter-particle collision times, and we predict these times by numerically solving a minimization problem. We have obtained results for dense random packs of various convex shapes such as cylinders, spherocylinders, and polyhedra, and we show results with these various particles packed together in a single pack to high packing fraction.

1. Introduction

Heterogeneous solid energetic materials are widely used in the aerospace and defense industries in rockets, explosives, and diverse pyrotechnic devices. The microstructure of these composites are often composed of particles of a crystalline oxidizer, such as ammonium perchlorate (AP) embedded in a polymer such as hydroxyl-terminated polybutadiene (HTPB) or polybutadiene acrylonitrile (PBAN). The polymers serve both as a binding agent and a fuel. Metal flake or powder, usually aluminum, may be added to increase the energetic content of the composite. Other composites may substitute crystals of an energetic material such as HMX for the oxidizer. Particle sizes for the composites range from a few μm for oxidizer particles in the “dirty binder” to 10s of μm for the metal flakes to 100s of μm for the largest oxidizer crystals. In explosives, the solids are loaded to mass fractions beyond 0.90, corresponding to volume fractions of 0.6–0.8. To achieve these high solids loadings, the materials are often compressed before the binder cures during manufacture. This results in particle breakage [1]. The final particle shapes are more polyhedral than spherical, but high aspect ratios seem to be rare [2]. Under conditions supporting deflagration, these composites burn with a reaction zone a few 100 μm thick. In certain scenarios, the deflagration can transition to a detonation [3]. Shown in Fig. 1 is a slice through an HMX-based explosive, illustrating the microstructure of a typical explosive. The HMX crystals range from a few μm to several hundred μm in size and are embedded in a rubbery binder.

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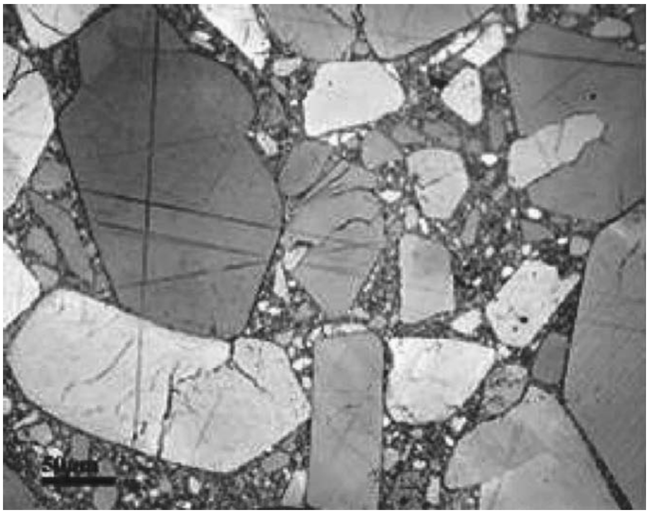

Fig. 1. A polarized light micrograph of a plastic bonded explosive (PBX) based on the energetic material HMX. The size scale is 50 μm. (Photo courtesy of C. Skidmore at LANL [43].)

Porous energetic materials are also common in the aerospace and defense industries, where the porosity is present either by choice, as in the case of rocket igniters, or by nature, as in the case of aging fractured explosives. These materials often also have heterogeneous microstructure, having been manufactured using the composites mentioned above. The grains in igniters and gun propellants are often characterized by a particular shape, such as perforated rods, spherocylinders, or prismatic stars, into which they have been pressed or cast. These grains are poured loosely or packed tightly into rigid containers such as gun shells. The size of propellant grains varies widely, from several 100s of μm to 10s of mm. Solids loading ranges from 50% to 70% by volume (the remainder is void space). The grains are often coated with deterrents that reduce the initial burn rate and enhance propellant performance [4–7]. Fractured energetic materials have significantly different properties than gun and igniter propellants, but they share some common porous material characteristics. The fractures develop over time as the explosive ages, increasing the porosity to the point that the overall device becomes unstable and unsafe. Because fractured explosive began life as solid composites, they typically exhibit much lower porosity than igniters and gun propellants, with volume fractions ranging from 0.7 to 1.0 [8]. In either case, these porous materials have macroscopic burn characteristics quite different than the solid composites [9].

Designers of devices using these materials are concerned with various properties of the materials as they relate to safety and engineering issues. These include thermo-mechanical properties such as Young's modulus, mechanical stability and thermal conductivity, as well as burn rate and metal agglomeration characteristics, among others. These bulk properties are strongly dependent on the morphology of the materials, and it is thus necessary to have a proper model for the morphology. Packs of disks and spheres have been extensively used for this purpose with much success. In particular the dependence of the burn rate on the morphology of composite AP/HTPB has been studied extensively using packs of spheres [10,11]. At least for burn rate studies, spheres appear to be a reasonable approximation to the shape of the particles, and a study of spheroids showed little dependence of burn rate on sphericity [12]. Likewise, much success has also been reported in aluminum agglomeration model development with packs of polydisperse spheres [13].

Nevertheless, spheres can be poor approximations to heterogeneous and porous materials when various other properties are of interest. Bulk material properties such as thermal conductivity [14] and elastic properties [15] strongly depend on the statistical details of the microstructure, and spheres do not properly replicate these statistics. Efforts to design a statistically optimal periodic unit cell as a model of the microstructure of a composite energetic material also depend on better approximations of the shape of the particulates [16].

Porous flow is another area where spheres may perform poorly as models of morphology. Understanding the fluid flow in porous energetic materials is crucial when designing explosive devices to ensure their proper operation and long term safety [6]. Fluid flow phenomena strongly affect burn rates in porous materials and may play a strong role in the detonation to deflagration transition (DDT) in energetic materials. DDT is an important topic for the safety and reliability of the nuclear stockpile [8]. As with the thermo-mechanical properties, fluid flow through porous energetic materials is also strongly dependent on the shape of the particle. For example, the well-known Ergun correlation for pressure drop through a packed bed is accurate for monodisperse spheres under many conditions and even works well for monodisperse packs of some non-spherical particles when the particle shape is adequately accounted for [17]. However, when used where the particles have large polydispersity or are moderately non-spherical, the Ergun relation fares poorly [18]. Other empirical correlations for the drag coefficient and permeability of a porous medium also work well for spheres, but fail for more complex structures. In one particularly relevant experiment, empirical relations for predicting the permeabilities of packed beds of spheres were found to over-predict the measured permeability of the non-spherical explosive CP by factors of 5–50 [19].