Thermodynamic approach to particle size distributions of complex particulate media: modelling and packing parameters.

Miguel Angel Martín[a]

[a] *Departamento de Matemática Aplicada, Escuela Técnica Superior de Ingenieros Agrónomos, TechnicalUniversityof Madrid, 28040 Madrid, Spain.*

Phone: +34 91 336 58 13, *Fax:* +34 91 336 5817 *E–mail address:* miguelangel.martin@upm.es

The study of particulate systems is of great interest in many fields of science and technology. Soil, sediments, powders, granular materials, colloidal and particulate suspensions are examples of systems involving many size particles. For those systems, the statistical description of the particle size distribution (PSD), that is, the mathematical distribution that defines the relative amounts of particles present, sorted according to size, is a crutial issue. The PSD can be important in understanding soil hydraulic properties, the geological origin or sediments or the physical and chemical properties of granular materials and ceramics, among others.

Several probability distributions have been used as PSD models depending on the nature of the particle system. The log-normal and Weibul distributions have been traditionally used for modelling particle size distributions generated by grinding, milling and crushing operations. The log-hyperbolic distribution was proposed in Bagnold and Barndof-Nielsen, 1980 to model PSD of naturally occurring sediments and a log-Laplace model was proposed in Fieller et. al. 1984 as an alternative for the same scenario. In Mandelbrot, 1982 and Turcotte, 1986 a connection between fractals and fragmentation was made being the start point of a number of studies using fractals to model complex size distributions in different systems and particularly in soil (see, for instance, Pachepsky et al. 2000 and Sornette, 2006).

On the other hand, the packing of particles affects to the physical properties of the granular system. Properties of particulate materials highly depend on the packing structure. Also the hydraulic properties (water retention) of granular porous media, as in the case of soil, depend on the bulk density and the geometric scale arrangement of the intergranular space. Even when the particles are modelled by hard spheres, and disregarding the filling material occupying the intergranular space, models of granular media can be useful in predicting different properties of a wide number of natural and engeniering systems as soil, ceramics, porous materials, concentrated suspensions, amorphous materials, alloys or microstructures of simple liquids. Because of that, the study of the random packing of particles has attracted researchers in many areas of science and technology (see Gray, 1968). In particular, the crutial influence of particle size distribution on the random packing structure increase the interest in relating both, either theoretically or by computational methods. Sohn and Moreland, 1968 studied the effect of Gaussian and lognormal distributions on packing density using dense random packing of sands, and Roualt and Assouling,1998 use a probabilistic approach to determine the distribution of the volumen of the voids in packed spheres once their size distribution is given. Anishchik and Medvedev, 1995 used a three-dimensional Apollonian packing as a model for dense granular systems investigating the particle size distribution and the fractal nature of packings. Packing of spheres with lognormal distributions by mean of computer simulation have been studied in Nolan and Kavanag,1993 and He et al.,1999 used a Monte Carlo simulation for a random model of spherical particles of sizes obbeing any given distribution.

Andreasen and Andersen, 1930 address together the modelling of PSD and the packing of particles of real granular media produced by grinding and involving particle sizes below a certain size. There, an original physicoempirical model with a mathematical formulation is proposed. The model and the ability to predict both, the PSD and the packing fraction, are tested using data obtained by materials and operations commonly used in ceramic industry. As far as this author know, the proposal of these kind of original models for PSD (beyond the simple testing of classical distributions) providing simultaneously packing parameters, are scarce.

The goal of this note is proposing a modelling of grain PSD on the basis of interpreting, under the point of view of Information Theory, features commonly observed in a wide number of real granular media. A fractal modeling of the PSD, essentially resting in primary principles, is achieved. It also allows to introduce a meaningful entropy like parameter as a candidate to drive packing in the context of those granular media. The spirit of this work agrees in several aspects with the pioneering work of Andreasen and Andersen, 1930. As a matter of fact, we focus the study in the same kind of particulate media, and persues similar objectives, here by applying concepts and tools of Statistical Mechanics and Information Theory.

.