EQUATIONS OF STATE IN SOIL COMPRESSION BASED ON STATISTICAL MECHANICS[i]

Discussion by IGNACIO G. TEJADA[ii] and RAFAEL JIMENEZ[iii]

The authors have published a very interesting contribution in which they present a new and general relationship between void ratio and overburden pressure in the compression process of soils. The study is based on the law of interparticle energy distribution used in statistical mechanics and, in particular, the compression process of a soil is described according to its initial and final void ratios, and to a parameter β which is related to the potential energy of a soil element. Such potential energy depends not only on the mass and elevation of soil particles, but also on the interactions between them. To account for such interactions, the authors introduce the concept of "imaginary particles", which allows them to use empirically-calibrated β values in the formulation without the need to consider interparticle interactions explicitly. In fact, the results presented by the authors show that such approach reproduces successfully the compression behaviour of a wide range of situations and soils.

The purpose of this discussion is to extend and clarify some theoretical aspects that might be helpful for a better understanding of Fukue and Mulligan's work. To that end, we build on the work of Edwards and Oakeshott (1989), who presented a study of how statistical mechanics applies to powders. We believe that there are some fundamental differences between both approaches that deserve some discussion, with the important conceptual conclusion that β should not depend on the product kT.

For an ideal gas, temperature and pressure are directly related to the kinetical energy of the gas molecules, and that makes the distribution of energy levels to depend on temperature. In a soil at equilibrium, however, particles are not in motion, pressure is related to forces transmitted between particles rather than to their movements, and temperature is related to the vibration of the atoms in the lattice of their structure rather than to their motion (which happens on a different scale). Such differences indicate that, for soil at equilibrium, the gravitational energy is much higher than thermal energy, which suggests that there are other variables (different to temperature) that have a much stronger influence on β. This idea is explained in detail below.

The total physical energy of a soil at equilibrium consists of both intraparticle energies (e.g., temperature, lattice energy, deformation energy, etc.) and of external energies, related to the arrangement of particles. At equilibrium, the external energies are only of potential type (e.g., gravitational, electrical, . . .) and, if particles are not crushing during compression of the soil, the expected energy change is only due to changes of the arrangement energy (since neither heat transfer nor change in the internal energy are expected). Therefore, although the 1st and the 2nd laws of thermodynamics are (of course) still valid, the amount of heat energy is negligible and the system is not governed by the typical equation state of a pVT system (such as an ideal gas). In this context, when Fukue and Mulligan describe the physical meaning of μ, they use the thermodynamical equation which expresses the change in internal energy, Eq. (28), but since in soil compression internal energy is hardly varied, this equation is probably not very adequate from a theoretical perspective.

This fundamental idea was considered by the statistical mechanics theory of powders developed by Edwards and Oekshott (1989). They argued that, in powders, it is their density (or, equivalently, their volume) which plays the role of energy in conventional statistical mechanics (i.e., as applied to ideal gases). Of course, both approaches should coincide, because potential and interaction energy are related to volume. They also defined the partition function (analogous to Eq. (25) in Fukue and Mulligan's work) in terms of volume and defined a sort of "entropy" and a sort of "temperature" that are mathematically similar to those used in thermodynamics but which have a different physical meaning. Table 1 in their paper elegantly summarizes the formal analogy between classical statistical mechanics and their formulation of statistical mechanics for powders.

It is important to note (*see* (35)) that, for ideal gases, the Boltzmann parameter is $e^{-H(q,p)/kT}$ (i.e., the exponential of the ratio between the Hamiltonian function and the product of the Boltzmann's constant by the temperature), whereas for powders it is $e^{-W(q)/\lambda X}$ (i.e., the exponential of the ratio between the compatible volume of the arrangement and the product of a constant, λ, by the frothiness, a concept which in soil mechanics is related to the size, shape and roughness of the particles). Such result illustrates how statistical mechanics can be employed to justify the well-known empirical observation that T is not (at least in the typical ranges of variation considered in civil engineering) a very significant parameter that affects the short-term behaviour of the soil; and that there are other parameters related to the intrinsic characteristics of soils (e.g., particle sizes, rough-

i) By Masaharu FUKUE and Catherine N. MULLIGAN, Vol. 49, No. 1, February 2009, pp. 99-114.

ii) PhD Student, ETSI de Caminos, Canales y Puertos, Universidad Politécnica de Madrid, Professor Aranguren S/N, 28040, Madrid, Spain (igtejada@caminos.upm.es).

iii) Senior Lecturer, ditto (rjimenez@caminos.upm.es).

ness, etc.) that have a stronger influence on the energy levels distribution and, therefore, on the compression behaviour. (It is expected that this approach based on the statistical mechanics theory of powders could avoid the need of the "imaginary particles" concept employed by Fukue and Mulligan.) Finally, it has to be emphasized again that the alternative approach proposed in this discussion (although perhaps more adequate from a theoretical perspective) does not limit the validity of Fukue and Mulligan's results, since they employed empirically-derived β values.

Reference

35) Edwards, S. F. and Oakeshott, R. B. S. (1989): Theory of powders, *Physica A.*, **157**, 1080–1090.