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Physical modeling of macroscopic properties of the complex many-particle, poly-dispersive micromechanical (granular) systems

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The study of the influence on the formation of macroscopic properties of multi-component mixtures is a complex and continuing to be an urgent task of fundamental physics and its numerous applications [1]. The traditional difficulties in determining reference states are supplemented by the difficulties of taking into account the effect of compaction in multicomponent mixtures. The task of describing the relationships between the micro- and macro-parameters of such systems is further complicated by the fact that multi-component mixtures (even if they are granular) can be in various states of aggregation from gaseous and liquid to crystalline.

Presented paper develops theoretical approaches to the description of macroscopic (compressibility) and structural (compaction) characteristics of complex many-particle, poly-dispersive multi-component mixtures, using Kirkwood-Buff's semi-phenomenological algorithm [2], molecular models like Carnahan-Starling-Mansoori [3]. Based on a comparative analysis would be build a prognostic base for the practical application of the results obtained in order to optimize (achieve the required values) of control parameters in liquid, granular mixtures by manipulation of their composition and/or compaction. Along this line, using the Carnahan–Starling–Mansoori hard-sphere conglomeration models and the Kirkwood–Buff statistical theory, the effect of compaction (packing) on the compressibility of a binary granular mixture has been analyzed [4]. The theoretical results are compared with the experimental ones obtained in alternative studies of the systems whose internal structure corresponds to the construction characteristics of the model [5]. The possibility of the maximum packing effect at special dispersion and mole fraction values of the components has been shown. The existence of the limit and intermediate states of the mixture with a predominant concentration of one of the components and the possibility of the most adequate description of the system properties in such states using one of the above-mentioned approaches have been demonstrated. The interval of values for the component volume fractions has been determined, where both approaches well describe the data of corresponding experiments.

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