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O.I. GERASYMOV, A.YA. SPIVAK

Odesa I.I. Mechnikov National University (2, Vsevoloda Zmiienka Str., Odesa 65082, Ukraine; e-mail: gerasymovoleg@gmail.com)

# PACKING AND COMPRESSIBILITY OF BINARY MICROMECHANICAL (GRANULAR) SYSTEMS

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. 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. 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.

 $\mathit{Keywords}$ : granular materials, mixtures, compaction, compressibility.

## 1. Introduction

The study of mechanical and other physical properties of micromechanical (granular) materials is a traditionally relevant subject of research in various domains of both experimental and theoretical physics. The presence of successful model approaches to describe some artificially constructed systems under specially created external conditions does not eliminate the problem associated with the absence of a general theory for physical processes in granular materials, which would allow the description of all physical phenomena and processes observed in them from a single viewpoint. The above concerns both the description of the observed structural formations and

the dynamics of transitions between states with different local symmetries. If we ignore the effects associated with dissipative interactions between the granules and the influence of the particle surface shape in large conglomerations of micromechanical (granulated) systems, then mono- and polydisperse systems consisting of hard spheres can serve as their rather productive model. The theory of the physical properties of such systems has been developed in detail; see, for example, [1–4].

Note that although the hard-sphere model does not provide a sufficient quantitative agreement between theoretical and experimental data, just in the case of granular materials, which are conglomerations of micromechanical particles, it enables the qualitative illustration of such physical phenomena as packing and compressibility.

In this paper, based on the statements of classical models of many-particle systems [3–5] and using the results of experimental studies performed in the work [6], we will show that, for a binary system of hard

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balls, the maximum compaction (packing) is possible, which is achieved by selecting the dispersion of components. We will also demonstrate that this type of non-monotonicity is qualitatively repeated for such a macroscopic property as compressibility. Thus, a relation between the local characteristics and macroscopic properties of examined systems will be demonstrated, which has similarity signs.

We will also demonstrate the similarities and differences between the results obtained while describing the compressibility of model binary mixtures using the Kirkwood–Buff (KB) [5] and Carnahan–Starling–Mansoori (KSM) [4] approaches and determine intervals, where either (or even both) of them can be applied most adequately. The KSM model is based on a semi-empirical equation of state for a system of hard spheres. The KB model is based on taking density fluctuations in multiparticle systems into account using correlation integrals.

# 2. Compressibility of a Two-Component Conglomerate of Hard Spheres. Carnahan-Starling-Mansoori Approach

The compressibility parameter is determined by the formula

$$\beta = -\frac{1}{V} \frac{\partial V}{\partial p} = \frac{1}{n} \frac{\partial n}{\partial p},\tag{1}$$

where V, p, and n are the volume, pressure, and concentration of the system, respectively. Also used is a quantity called the compactness – the compactness (or packing) parameter – which is determined by the formula

$$\eta = nv_0, \tag{2}$$

where  $v_0$  is the volume occupied by one individual particle. In particular, for spherical granules,  $v_0 = \frac{1}{6}\pi\sigma_0^3$ , where  $\sigma_0$  is the particle diameter.

In the work [4], it was shown that the compressibility of a binary multi-particle mixture of hard spheres can be represented in the following form:

$$\beta_T^{(1,2)} = \frac{1}{n_{12}k_{\rm B}T} \frac{(1-\eta)^4}{1+a\eta+b\eta^2+c\eta^3+d\eta^4},\tag{3}$$

where 
$$\eta \equiv \eta_{12} = \frac{1}{6} \pi n_{12} \sigma_{12}^3$$

is the compaction parameter of the binary mixture (with components 1 and 2),  $n_{12}$  is the particle concentration for the binary mixture, and  $\sigma_{12}$  is the effective size. The latter can be determined through the mole fraction x,

$$\sigma_{12}^3 = (1-x)\sigma_1^3 + x\sigma_2^3$$

or through the volume fraction f,

$$\sigma_{12}^3 = \frac{\sigma_1^3 \sigma_2^3}{(1-f)\sigma_2^3 + f\sigma_1^3},$$

where  $\sigma_1$  and  $\sigma_2$  are the hard-sphere diameters of the mixture components; the coefficients a, b, c, and d depend on the component mole fraction x in the mixture (or their volume fraction  $f = V_S/(V_L + V_S)$ , where  $V_L$  and  $V_S$  are the volumes of the fractions consisting of large and small particles, respectively), and on the particle size ratio  $r = \sigma_1/\sigma_2$ .

As shown in [4], these coefficients are determined using the following expression:

$$a = 4 - 6y_1, \quad b = 4 - 3y_1 - 9y_2,$$
  
 $c = -4y_3, \quad d = y_3,$ 

$$(4)$$

where  $y_1, y_2,$  and  $y_3$  look like

$$y_1 = \Delta \cdot \left(\sqrt{r} + \frac{1}{\sqrt{r}}\right),\tag{5}$$

$$y_2 = \Delta \cdot \left( f\sqrt{r} + \frac{1-f}{\sqrt{r}} \right), \tag{6}$$

$$y_3 = [(1-f)^{2/3} \cdot (1-x)^{1/3} + f^{2/3} \cdot x^{1/3}]^3,$$
 (7)

$$\Delta = \sqrt{f(1-f)x(1-x)} \cdot \left(\sqrt{r} - \frac{1}{\sqrt{r}}\right)^2. \tag{8}$$

Note that the ratio between the volume and mole fractions and the size ratio x are given by the following formulas:

$$f = \frac{x}{r^3 - (r^3 - 1)x}, \quad x = \frac{r^3 f}{1 + (r^3 - 1)f},\tag{9}$$

where 
$$r^3 = \frac{x}{1-x} \, \frac{1-f}{f}.$$

Using the Carnahan–Starling–Mansoori formula (3), we numerically calculated the coefficient  $n_{12}k_{\rm B}T\beta_T^{(1,2)} \equiv \chi_{12}$  by varying the size ratio r, the volume fraction f, and the compaction parameter  $\eta$ . The

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results obtained are presented as a 3-dimensional phase diagram in Fig. 1. From this figure, it follows that the coefficient  $\chi_{12}$  has a distinctly pronounced maximum whose amplitude increases, whereas the width decreases, with the growth of the mixture dispersion factor (the ratio r between the sizes of the spheres). In particular, the maximum shown in Fig. 1, a (for  $r \approx 9$ ) is high and narrow, but it is lower and smoother in Fig. 1, b (for  $r \approx 2$ ). The numerical values of the compressibility coefficient decrease as the compaction parameter increases. The position of the maximum also shifts from  $f \approx 0.5$  (for small size ratios between the mixture components,  $r \approx 1$ ) to  $f \rightarrow 0$  (for larger r-values,  $r \gg 1$ ).

# 3. Calculation of the Coefficient $\chi_{12}$ for Measured Compaction $\eta_{12}$ -Values [6]

In the work [6], a binary mixture of hard spherical balls with different sizes was experimentally studied. The size ratio was varied within the interval  $r\approx 2\div 35$ . As the main result obtained in [6], we may consider non-monotonic dependences of the compaction parameter and the diameter ratio between the binary mixture components on the component volume fraction, with characteristic maximums.

Using the Carnahan–Starling–Mansoori formula (3), we numerically calculated the quantity  $n_{12}k_{\rm B}T\beta_T^{(1,2)}$  at the same values of the particle size ratio ( $r\approx 2\div 35$ ) that were used when measuring the compaction in the work [6]. In so doing, the corresponding values of the mixture compaction  $\eta$  measured in [6] were used self-consistently. The results obtained are presented in Figs. 2–5 as 2-dimensional phase diagrams.

The dependences of the compressibility coefficient  $\chi_{12}$  on the coefficient r characterizing the dispersion of the components, which are plotted in Fig. 2, distinctly demonstrate the presence of specific states in the behavior of this parameter. Namely, two characteristic types of behavior can be distinguished: (a) a sharp increase of  $\chi_{12}$  with the growth of r (the curves were plotted for the volume fraction within the interval  $0.05 \leq f \leq 0.20$ ) and (b) slow changes of  $\chi_{12}$  as r increases (the curves were plotted for the volume fraction within the interval  $0.25 \leq f \leq 1$  and for f=0). Such a difference in the behaviors of  $\chi_{12}$  can be considered as a result of different states of the corresponding local structure. In the theoretical work

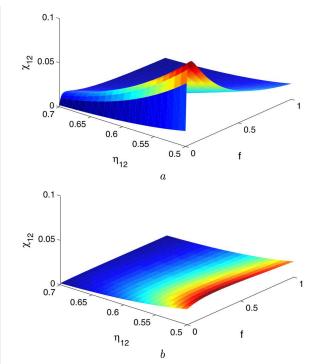


Fig. 1. Dependences of the compressibility coefficient  $\chi_{12}$  on the mixture compaction parameter  $\eta_{12}$  and the volume fraction f calculated by formula (3) for  $r \approx 9$  (a) and  $r \approx 2$  (b)

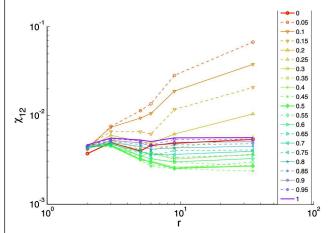


Fig. 2. Dependences of the compressibility coefficient  $\chi_{12}$  on the dispersion coefficient r calculated by formula (3) using the parameters from the experimental work [6]. The dispersion coefficient r changes within the interval  $r\approx 2\div 35$ . The volume fraction f was varied with the step  $\Delta f=0.05$  within the full possible interval  $f=0\div 1$ 

[8], those states were proposed to call "gravel" for  $f \ll 1$  and "pudding" for  $(1-f) \ll 1$ . In these terms, the behavior of type (a) is typical of the "gravel"

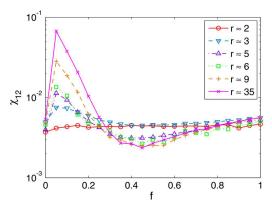


Fig. 3. Dependences of the compressibility coefficient  $\chi_{12}$  on the volume fraction f calculated by formula (3) using the parameters from the experimental work [6]. The dispersion coefficient r changes within the interval  $r\approx 2\div 35$ . For each plot, the volume fraction f was varied with the step  $\Delta f=0.05$  within the full possible interval  $f=0\div 1$ 

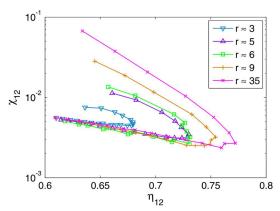


Fig. 4. Dependences of the compressibility coefficient  $\chi_{12}$  calculated by formula (3) using the parameters from the work [6]  $(r \approx 3 \div 35)$ 

state, and the behavior of type (b) is typical of the "pudding" state.

The dependences of the compressibility coefficient  $\chi_{12}$  on the volume fraction f plotted in Fig. 3 also demonstrate the presence of the above-mentioned limit states. Namely, (a) a sharp maximum of  $\chi_{12}$  for the volume fraction within an interval of  $0 \le f \le 0.20$  and (b) a wide minimum of  $\chi_{12}$  for the volume fraction values within an interval of  $0.25 \le f \le 1$ . Such a behavior of  $\chi_{12}$  can also be interpreted as the presence of the aforementioned "gravel" and "pudding" states. Accordingly, the extremum of the maximum type shown in Fig. 3 may correspond to the "gravel" state, and the extremum of the minimum type to the "pudding"

one. As the dispersion coefficient r increases, the determined extrema of  $\chi_{12}$  behave differently: the maximum increases by amplitude, whereas the minimum initially increases, but later this growth terminates (saturates).

The results shown in Fig. 4 demonstrate the dependences of the compressibility coefficient  $\chi_{12}$  on the compaction parameter  $\eta_{12}$  calculated using formula (3) for the same values of the parameter r ( $r \approx 2 \div 35$ ) as in the work [6]. According to the classification of states for a bidisperse granular mixture proposed in the work [8], their presence can also be detected with the help of the data presented in Fig. 4: the upper branches of the loop diagrams correspond to the "gravel" phase, and the lower ones to the "pudding" phase.

A pronounced asymmetry of the transition region is observed in Fig. 4. It is this region, which characterizes the transition between the selected limit phases (on the phase diagram), that was described in [8] as conditionally existing.

# 4. Compressibility of a Binary System of Hard Spheres According to the Kirkwood–Buff Theory [5]

The classical Kirkwood-Buff formula for a mixture of two components (marked as 1 and 2), which describes its isothermal compressibility  $\beta_T^{(1,2)}$ , looks like [5]

$$\beta_T^{(1,2)} = \frac{1}{k_{\rm B}T} \times \frac{1 + n_1 G_{11} + n_2 G_{22} + n_1 n_2 (G_{11} G_{22} - G_{12}^2)}{n_1 + n_2 + n_1 n_2 (G_{11} + G_{22} - 2G_{12})}, \quad (10)$$

where  $n_1 = \frac{N_1}{V}$  and  $n_2 = \frac{N_2}{V}$  are the partial particle concentrations;  $G_{11}$ ,  $G_{22}$ , and  $G_{12}$  are the so-called correlation integrals; and  $k_{\rm B}T$  is the energy scale.

The correlation integrals  $G_{\alpha\beta}$  are related to the partial structure factors  $S_{\alpha\beta}(0)$  via the following relationships:

$$S_{\alpha\beta}(0) = x_{\alpha}\delta_{\alpha\beta} + x_{\alpha}x_{\beta}n_{12}G_{\alpha\beta},\tag{11}$$

where  $x_{\alpha}$  and  $x_{\beta}$  are the mole fractions of the mixture components;  $\delta_{\alpha\beta}$  is the Kronecker delta symbol, and  $n_{12} = \frac{N}{V} = \frac{N_1 + N_2}{V} = n_1 + n_2$  is the mixture concentration. Using formula (11), it is easy to obtain that

$$S_{11}(0) = (1-x) + (1-x)^2 n_{12} G_{11}, (12)$$

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$$S_{22}(0) = x + x^2 n_{12} G_{22}, (13)$$

$$S_{12}(0) = x(1-x)n_{12}G_{12}, (14)$$

where x is the mole fraction of component 2 in the mixture. Substituting relationships (12)–(14) into the Kirkwood–Buff formula (10), we obtain the relationship between the isothermal compressibility of a binary mixture and the partial factors  $S_{\alpha\beta}(0)$  in the following form:

$$\beta_T^{(1,2)} = \frac{1}{n_{12}k_BT} \times \frac{S_{11}(0)S_{22}(0) - S_{12}^2(0)}{x^2S_{11}(0) + (1-x)^2S_{22}(0) - 2x(1-x)S_{12}(0)}.$$
 (15)

Taking into account that the factor S(0) of a monodisperse system is determined as follows:

$$S(0) = 1 + nG = nk_{\rm B}T\beta_T,\tag{16}$$

as well as Eqs. (12) and (13), we obtain the following expressions for the partial factors of monodisperse phases  $S_{11}(0)$  and  $S_{22}(0)$  with the partial isothermal compressibilities  $\beta_T^{(1)}$  and  $\beta_T^{(2)}$ :

$$S_{11}(0) = (1 - x) \cdot n_1 k_{\rm B} T \beta_T^{(1)}, \tag{17}$$

$$S_{22}(0) = x \cdot n_2 k_{\rm B} T \beta_T^{(2)}. \tag{18}$$

The partial (reference) isothermal compressibilities  $\beta_T^{(1)}$  and  $\beta_T^{(2)}$  can be determined, for example, using model equations of state. Using data on the isothermal compressibility of the mixture  $\beta_T^{(1,2)}$ , which can be taken from alternative sources (for example, from experiments or carrying out numerical simulations), and solving Eq. (15) with respect to the factor  $S_{12}(0)$ , we obtain

$$S_{12}(0) = x(1-x) \cdot \chi_{12}^{KB} \pm \left\{ x^2 (1-x)^2 (\chi_{12}^{KB})^2 - \chi_{12}^{KB} \left[ x^2 S_{11}(0) + (1-x)^2 S_{22}(0) \right] + S_{11}(0) S_{22}(0) \right\}^{1/2},$$
where  $\chi_{12}^{KB} = \pi_{12} L T \ell^{(1,2)}$  (19)

where  $\chi_{12}^{\text{KB}} = n_{12}k_{\text{B}}T\beta_{T}^{(1,2)}$ . In the work [6], experimental data were obtained for the compaction of a binary mixture of spherical particles with various size difference for  $r \approx 2 \div 35$ . The obtained data were actually parametrized in two characteristic limits (states) of the mixture where the content of either larger ("gravel") or smaller ("pudding") particles prevails. In the work [7], an attempt

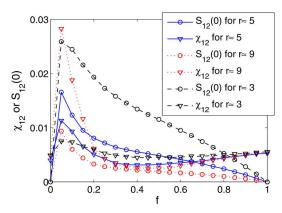


Fig. 5. Dependences of the compressibility coefficient  $\chi_{12}$  on the volume fraction f calculated by formulas (3) and (19) using the parameters from the experimental work [6]. The dispersion coefficient r changes within the interval  $r \approx 3 \div 9$ . For each plot, the volume fraction f was varied with the step  $\Delta f = 0.05$  within the full possible interval  $f = 0 \div 1$ 

was made to describe the experimental data obtained in all intermediate states by extrapolating the phenomenological relationships, which were obtained only for the limit states, with the help of weight functions playing the role of undetermined (actually, fitting) parameters. Moreover, these fconcernunctions only the limit states and remain consistently undetermined at the intermediate ones.

In Fig. 5, the results of our numerical calculations obtained for the dependences of the compressibility coefficient  $\chi_{12}$  and the structural factor  $S_{12}(0)$ on the volume fraction f are exhibited. The compressibility coefficient  $\chi_{12}$  was calculated by formula (3) according to the Carnahan–Starling–Mansoori model equation of state for a binary system of hard spheres [4], and the structural factor  $S_{12}(0)$  was calculated by formula (19) obtained using the Kirkwood-Buff theory [9, 10]. The  $\chi_{12}$ - and  $S_{12}(0)$ -plots intersect at two points. One of them is in the interval of small volume fractions of one of the mixture components, and the other in the interval where it takes the largest possible values. They can be interpreted as the separation of two states in the mixture with the same compaction but different component compositions. The concentration of larger particles ("gravel") prevails in the first state, and the concentration of smaller particles ("gravel") prevails in the second one.

For illustrative purposes, only selected values of the dispersion coefficient  $(r \approx 3 \div 9)$  are used in Fig. 5.

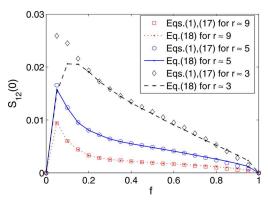


Fig. 6. Dependences of the quantity  $S_{12}(0)$  on the volume fraction f calculated by formulas (19) and (20) using the parameters from the experimental work [6] for some values of the component size ratio r within the interval  $r \approx 3 \div 9$ 

- Let the fine component dominate in the mixture. Then, at  $r \approx 5$ , we have that  $S_{12}(0) = \chi_{12}$  at the volume fraction  $f \approx 0.65$ ; at  $r \approx 3$ , we have that  $S_{12}(0) = \chi_{12}$  at the volume fraction  $f \approx 0.81$ . Thus, as the value of the dispersion coefficient r increases, the value of the volume fraction f at which  $S_{12}(0) = \chi_{12}$  (the "pudding" state) decreases.
- Let the coarse component dominate in the mixture. Then, at  $r \approx 5$ , we have that  $S_{12}(0) = \chi_{12}$  at the volume fraction  $f \approx 0.011$ ; for  $r \approx 3$ , we have that  $S_{12}(0) = \chi_{12}$  at the volume fraction  $f \approx 0.025$ . Thus, as the value of the dispersion coefficient r increases, the value of the volume fraction f at which  $S_{12}(0) = \chi_{12}$  (the "gravel" state) also increases.

Thus, with the increase in the dispersion coefficient r, the value of the volume fraction f, at which  $S_{12}(0) = \chi_{12}$ , (the "gravel" state) increases.

It can be shown that, for  $r \approx 9$  and  $r \approx 35$ , the  $S_{12}(0)$ - and  $\chi_{12}$ -plots do not intersect at all. The absence of intersection points of the  $S_{12}(0)$ - and  $\chi_{12}$ -functions coincides with the existence of the critical dispersion coefficient value  $r_c = 3 + \sqrt{12} \approx 6.46$ , which was found in the work [6]. One of the qualitative explanations is as follows. As the dispersion of mixture components grows starting from the  $r_c$ -value, the probability that the particles of the fine component can slip through the gaps formed by, say, three densely packed particles of the coarse component and fill a new free volume that was previously inaccessible for them increases, which changes the compaction and, as a consequence, can change the mixture properties (for example, as shown in [6], the packing rate).

The existence of some critical size difference between the components, which was experimentally discovered in [6] and obtained theoretically by us, manifests itself by its influence on the compaction rate and is responsible for the principle possibility of obtaining the maximum and minimum values of this parameter. Hence, for a mixture with  $r < r_c$ , it is possible to use formula (3) where the coefficient  $n_{12}k_{\rm B}T\beta_T^{(1,2)}$  is proportional to  $S_{12}(0)$  (strictly speaking, this can be done at separate points, provided the self-consistently determined values of the volume fraction f). If  $r > r_c$ , we cannot assume the proportionality between the coefficient  $n_{12}k_{\rm B}T\beta_T^{(1,2)}$  in formula (3) and  $S_{12}(0)$ .

Note also that, by postulating the replacement of the coefficient  $n_{12}k_{\rm B}T\beta_T^{(1,2)}$  by the function  $S_{12}(0)$  in the Kirkwood–Buff formula (15)–recall that the function  $S_{12}(0)$  was found in view of the previously established possibility that the coefficient  $\chi_{12}$  and the factor  $S_{12}(0)$  can coincide—and solving the corresponding quadratic equation with respect to  $S_{12}(0)$ , we obtain the following formula:

$$S_{12}(0) = \frac{x^2 S_{11}(0) + (1-x)^2 S_{22}(0)}{2[1 - 2x(1-x)]} \times \left\{ -1 + \sqrt{1 + \frac{4[1 - 2x(1-x)]S_{11}(0)S_{22}(0)}{[x^2 S_{11}(0) + (1-x)^2 S_{22}(0)]^2}} \right\}. \quad (20)$$

In Fig. 6, the plots of the dependences of  $S_{12}(0)$  on the volume fraction f calculated using expression (20) are compared with the analogous dependences calculated using formula (19).

As follows from Fig. 6, the dependence of  $S_{12}(0)$ on the volume fraction f determined in the way described above is non-monotonic; namely, it contains a well-pronounced maximum. An increase in r diminishes the amplitude of the  $S_{12}(0)$  maximum and shifts it toward smaller f-values. The plotted dependences demonstrate the following relationships between the  $S_{12}(0)$ -values calculated by formulas (19) and (20): they almost coincide at  $r \approx 9$ , are qualitatively similar at  $r \approx 6$ , and are strongly different at  $r \approx 3$ . Discrepancies are observed when the mixture composition approaches the monodisperse limits  $(f \to 0 \text{ and } f \to 1)$ . In the interval of volume fraction values  $f \approx 0.2 \div 0.8$ , an almost complete coincidence of the  $S_{12}(0)$ -behavior is observed for all approaches used for its determination.

#### 5. Conclusions

Taking the aforesaid into account, we come to the conclusion that the application of the Carnahan-Starling-Mansoori and Kirkwood-Buff models of binary mixtures of hard spheres, which are effectively used in molecular physics to describe the compressibility properties of real granular materials, showed the nonmonotonic dependence of this parameter on the size ratio and the mole fractions of the components. In particular, two characteristic states characterized by the dominant concentrations of either of the components (which we, following the work [8], call the gravel and pudding phases) and a transition region where the compressibility coefficient reaches its maximum values can be distinguished. The availability of the compressibility coefficient maximum at certain volume fraction values makes it possible to characterize and consistently describe (for example, in the form of corresponding phase diagrams) the existence of a transition zone in its behavior, which separates the limit states (pudding and gravel) with the prevailing concentrations of either of the mixture components. Moreover, it is important to note that the presence of the compressibility coefficient maximum, which we have established theoretically, correlates with a similar, experimentally revealed behavior of the compaction factor [6]. Such a behavior, although found at the model level, can help us to determine the compaction values at which the compressibility coefficient calculated by formulas (3) reaches its maximum and limit values. The intervals of the binary mixture parameters (the limit states) at which only one of the KSM [4] and KB [5] approaches used to describe the mixture compressibility is applicable have been determined, as well as the intermediate regions both of them can be applied quite adequately, which is confirmed by the data of the corresponding experimental measurements [6].

- M.S. Wertheim. Exact solution of the Percus-Yevick integral equation for hard spheres. Phys. Rev. Lett. 10, 321 (1963).
- E. Thiele. Equation of state for hard spheres. J. Chem. Phys. 39, 474 (1963).

- N.F. Carnahan, K.E. Starling. Equation of state for nonattracting rigid spheres. J. Chem. Phys. 51, 635 (1969).
- G.A. Mansoori, N.F. Carnahan, K.E. Starling, T.W. Leland, Jr. Equilibrium thermodynamic properties of the mixture of hard spheres. J. Chem. Phys. 54, 1523 (1971).
- J.G. Kirkwood, F.P. Buff. The statistical mechanical theory of solutions. I. J. Chem. Phys. 19, 774 (1951).
- S. Pillitteri, G. Lumay, E. Opsomer, N. Vandewalle. From jamming to fast compaction dynamics in granular binary mixtures. Sci. Rep. 9, 7281 (2019).
- S. Pillitteri, G. Lumay, E. Opsomer, N. Vandewalle. How size ratio and segregation affect the packing of binary granular mixtures. Soft Matt. 16, 9094 (2020).
- T. Boutreux, P.G. de Gennes. Compaction of granular mixtures: a free volume model. *Physica A* 244, 59 (1997).
- O. Gerasymov, A. Spivak, I. Andrianova, L. Sidletska, V. Kuryatnikov, A. Kilian. Micro-mechanical (granular) mixtures for environmental safety technologies. *E3S Web* of Conferences 234, 00075 (2021).
- O. Gerasymov, I. Andrianova, A. Spivak, L. Sidletska, V. Kuryatnikov, A. Kilian. Tightening (compaction) of bicomponent micromechanical (granular) system. Sci. Innovat. 17, 79 (2021). Received 26.02.25.

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### О.І. Герасимов, А.Я. Співак

## ВПАКУВАННЯ ТА СТИСЛИВІСТЬ БІКОМПОНЕНТНИХ МІКРОМЕХАНІЧНИХ (ГРАНУЛЬОВАНИХ СИСТЕМ

Із використанням моделей конгломерацій твердих сфер Карнахана-Старлінга-Мансурі та статистичної теорії Кірквуда-Баффа досліджується вплив компактизації (впакування) на стисливість бінарної гранульованої суміші. Теоретичні результати порівнюються з експериментальними, отриманими в альтернативних дослідженнях на системах, внутрішня структура яких відповідає конструктивним характеристикам моделі. Показано можливість існування ефекту максимального впакування при спеціальних значеннях дисперсії і мольної фракції компонентів. Продемонстровано існування граничних і проміжних станів суміші з переважною концентрацією одного із компонентів та показано можливість найбільш алекватного опису властивостей системи в цих станах за допомогою одного із вищезгаданих підходів. Виділено область значень об'ємної частки компонентів, в якій обидва підходи тотожні та добре описують дані відповідних експериментів.

Kлючові cлова: гранульовані матеріали, суміші, компактизація, стисливість.