Advances in Complex Systems

LIQUID-SOLID TRANSITION IN BIDISPERSE GRANULATES

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Simulation results of dense granulates with particles of different size are compared with theoretical predictions concerning the mixture pressure. An effective correlation function is computed which depends only on the total volume fraction and on the dimensionless width of the size-distribution function. From simulation data of elastic and weakly dissipative systems, one can predict how much disorder (size-dispersity) is necessary to avoid ordering effects due to crystallization. Finally, a *global equation of state* is proposed, which unifies both the dilute, disordered gas/fluid and the dense, solid regime.

1. Introduction

The hard-sphere (HS) system is a traditional and simple toy-model for various phenomena like e.g. disorder-order transitions, the glass transition, or simple gases and liquids [1–4]. A theory that describes the behavior of rigid particles in the gas and disordered fluid regime is the kinetic theory [1, 5], where particles are assumed to be rigid and collisions take place in zero time (they are instantaneous), exactly like in the hard-sphere model. In a more dense system which resembles a solid or a glass, particle-in-cell models or a free volume theory can be applied [6, 7]. In the intermediate transition regime, no satisfactory theoretical description is available at the moment [7–10].

When dissipation is added to the HS model, one has the inelastic hard sphere (IHS) model, i.e. the simplest version of a granular gas, a member of the more general class of dissipative, non-equilibrium, multi-particle systems [4, 11]. Attempts to describe granular media by means of kinetic theory are usually restricted to certain limits like constant or small density or weak dissipation [12–16]. In general, granular systems consist of particles with different sizes and properties, a situation which is rarely addressed theoretically [17–19]. However, the treatment of bi- and polydisperse mixtures is easily performed by means of numerical simulations [10, 20–22].

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In this study, theories and simulations for situations with particles of equal and different sizes are compared. In section 2, the model system is introduced and, in section 3, theoretical results are reviewed and compared with numerical results concerning the pressure. The disorder-order transition and the amount of difference in particle size, necessary to avoid it, is discussed in section 4. The results are summarized and discussed in section 5.

2. Model system

For the numerical modeling of the system, periodic, two-dimensional (2D) systems of volume $V = L_x L_y$ are used, with horizontal and vertical size L_x and L_y, respectively. N particles are located at positions $\boldsymbol{r}_i$ with velocities $\boldsymbol{v}_i$ and masses m_i. From any simulation, one can extract the kinetic energy $E(t) = \frac{1}{2}\sum_i m_i \boldsymbol{v}_i^2$, dependent on time via the particle velocity $\boldsymbol{v}_i = \boldsymbol{v}_i(t)$. In 2D, the "granular temperature" is defined as $T = E/N$.

2.1. *Polydispersity*

The particles in the system have the radii a_i randomly drawn from mono-, bi-, and polydisperse size distribution functions

$$w(a) = \begin{cases} \delta(a-a_0) & \text{with } \langle a \rangle = a_0 \\ n_1\delta(a-a_1) + n_2\delta(a-a_2) & \text{with } \langle a \rangle = (n_1 + (1-n_1)/R)a_1 \\ \frac{1}{2w_0a_0}\theta_{[(1-w_0)a_0,(1+w_0)a_0]}(a) & \text{with } \langle a \rangle = a_0 \end{cases} ,$$

with the two-sided step-function $\theta_{[x_1,x_2]}(x) = 1$ for $x_1 \le x \le x_2$ and $\theta(x) = 0$ otherwise.

In the bidisperse case, the number fractions are $n_1 = N_1/N$ for particles with size a_1 in a system with $N = N_1 + N_2$ particles in total and N_2 particles with radius a_2. The size ratio $R = a_1/a_2$ is needed to classify a bidisperse size distribution with the volume fraction $\nu = \nu_1 + \nu_2$ as the last relevant system parameter, since the partial volume fractions can be expressed in terms of n_1 and R. The dimensionless k-th moment is $A_k = n_1 + (1-n_1)R^{-k} = \langle a^k \rangle / a_1^k$, scaled by a_1.

Since needed later on, the expectation values for the moments of a and their combination, the dimensionless width-correction $\mathcal{A} = \langle a \rangle^2 / \langle a^2 \rangle$, are summarized in table 2.1 in terms of a_1, n_1, and R for the bidisperse situations and in terms of a_0 and w_0 in the polydisperse cases. Different values of ν are realized by shrinking or growing either the system or the particles.

		$\langle a \rangle$	$\langle a^2 \rangle$	$\langle a \rangle^2 / \langle a^2 \rangle$
(i)	monodisperse	a_0	a_0^2	1
(ii)	bidisperse	$A_1 a_1$	$A_2 a_1^2$	A_1^2/A_2
(iii)	polydisperse	a_0	$(1 + w_0^2/3)\, a_0^2$	$3\ /\ (3 + w_0^2)$

Tab. 2: Moments $\langle a \rangle$, $\langle a^2 \rangle$ and $\mathcal{A} = \langle a \rangle^2 / \langle a^2 \rangle$ of the size distribution functions

2.2. *Particle interactions*

The particles are assumed to be perfectly rigid and follow an undisturbed straight trajectory until a collision occurs as described below. Due to the rigidity, collisions occur instantaneously, so that an event driven simulation method [23, 24] can be used. Note that no multi-particle contacts can occur in this model.

A change in velocity – and thus a change in energy – can occur only at a collision. The standard interaction model for instantaneous collisions of particles with radii a_i, mass $m_i = (4/3)\pi\rho a_i^3$, and material density ρ is used in the following. (Using the mass of a sphere is an arbitrary choice.) The post-collisional velocities $\boldsymbol{v}'$ of two collision partners in their center of mass reference frame are given, in terms of the pre-collisional velocities $\boldsymbol{v}$, by $\boldsymbol{v}'_{1,2} = \boldsymbol{v}_{1,2} \mp \frac{(1+r)\ m_{12}}{m_{1,2}} \boldsymbol{v}_n$, with $\boldsymbol{v}_n \equiv [(\boldsymbol{v}_1 - \boldsymbol{v}_2) \cdot \hat{\boldsymbol{n}}]\, \hat{\boldsymbol{n}}$, the normal component of the relative velocity $\boldsymbol{v}_1 - \boldsymbol{v}_2$, parallel to $\hat{\boldsymbol{n}}$, the unit vector pointing along the line connecting the centers of the colliding particles, and the reduced mass $m_{12} = m_1 m_2/(m_1 + m_2)$. If two particles collide, the change of the translational energy is $\Delta E = -m_{12}(1 - r^2) v_n^2/2$.

3. Simulation and theory

In the following, we examine situations with different polydispersity. Most of the simulations were performed in the elastic limit, $r = 1$, however, we checked that also simulations with weak dissipation and some weak driving force lead to the same results. Due to the scaling of the pressure with the energy of the system, as introduced below, also homogeneously cooling situations [25] are well fitted by the elastic results, if the factor 2 is replaced by $(1+r)$. A more detailed discussion of the range of applicability of the elastic results with respect to density and dissipation-strength is far from the scope of this study.

3.1. *Particle correlations*

In **monodisperse systems**, the particle-particle pair correlation function at contact

$$g_4(\nu) = \frac{1 - 7\nu/16}{(1-\nu)^2} - \frac{\nu^3/16}{8(1-\nu)^4} \ , \tag{3.1}$$

can be derived theoretically from a low density expansion [1, 3, 7, 13, 24], and it depends on the volume fraction only. The first term of g_4 is denoted as $g_2 = (1 - 7\nu/16)/(1-\nu)^2$, on which the polydisperse equations are based, see below. The particle-particle correlation function as a function of the distance is obtained from the simulations by averaging over several snapshots, normalized to the value $g(r \gg 2a) = 1$ for long distances [10]. At densities around $\nu_c \approx 0.7$, a disorder-order transition is evidenced, where the ordered regime, $\nu > \nu_c$ is not described by Eq. (3.1). For some data and a more detailed discussion of $g(r)$, see Refs. [7, 10].

For **bidisperse situations**, the correlation functions g_{11}, g_{22}, and g_{12} are different for different species combinations [10]. The mixed correlation functions [10, 17], are here expressed in terms of $A_{1,2}$, R, and ν:

$$g_{11} = \frac{1-\nu\left(1-\frac{9}{16}\frac{A_1}{A_2}\right)}{(1-\nu)^2} \ , \tag{3.2}$$

$$g_{22} = \frac{1-\nu\left(1-\frac{9}{16R}\frac{A_1}{A_2}\right)}{(1-\nu)^2} \ , \quad \text{and} \tag{3.3}$$

$$g_{12} = \frac{1-\nu\left(1-\frac{9}{8(1+R)}\frac{A_1}{A_2}\right)}{(1-\nu)^2} \ . \tag{3.4}$$

Note that all g_{ij} are identical to $g_2(\nu)$ in the monodisperse case with $R = 1$ and $A_1 = A_2 = 1$. Within the statistical error, agreement between the theoretical predictions and simulation results is obtained [10].

The particle correlation functions from **polydisperse mixtures** are smooth functions with much less variety in magnitude than in the mono- and bidisperse situations. Interestingly, they resemble the distribution function of a gas or liquid with a smooth interaction potential [3].

Note that there is no indication of long range order even for the highest densities if the size distribution (bi- or polydisperse) is sufficiently wide, as discussed later in section 4.

3.2. *Stress and the equation of state*

The stress tensor, defined for a test-volume V, has two contributions, one from the collisions and the other from the translational motion of the particles. Using a and b as indices for the cartesian coordinates one has the components of the stress tensor

$$\sigma^{ab} = \frac{1}{V}\left[\sum_i m_i v_i^a v_i^b - \frac{1}{\Delta t}\sum_n \sum_{j=1,2} \Delta p_j^a \ell_j^b\right] \ , \tag{3.5}$$

with ℓ_j^b, the components of the vector from the center of mass of the two colliding particles j to their contact points at collision n, where the momentum Δp_j^a is exchanged. The sum in the left term runs over all particles i, the first sum in the right term runs over all collisions n occuring in the time-interval Δt, and the second sum in the right term concerns the collision partners of collision n – in any case the corresponding particles must be inside the averaging volume V. The mean pressure $p = (\sigma_1 + \sigma_2)/2$, with the eigenvalues σ_1 and σ_2 of the stress tensor, is now obtained from the simulations for different volume fractions [10].

In the monodisperse system, we obtain crystallization around $\nu_c = 0.7$, and the data clearly deviate from P_0, i.e. the pressure is strongly reduced due to crystallization and, thus, enhanced free volume. The monodisperse data diverge at the maximum packing fraction $\nu_{\rm max}^{\rm mono} = \pi/(2\sqrt{3})$ in 2D. The deviations of the polydisperse simulations increase with the width of $w(a)$ and with increasing volume fraction. Note that there exists a deviation already for small $\nu \to 0$.

3.3. *Mixture pressure*

A more elaborate calculation in the style of Jenkins and Mancini [17], leads to the partial translational pressures $p_i^t = n_i E/V$ for the species i and to the collisional pressures $p_{ij}^c = \pi N_i N_j g_{ij} a_{ij}^2 (1+r_{ij}) T/(4V^2)$. In elastic simulations, the species temperatures are equal, so that the corresponding correction term can be dropped. Thus, the global mixture pressure is

$$\begin{aligned} p^{\mathrm{m}} &= p_1^t + p_2^t + p_{11}^c + 2p_{12}^c + p_{22}^c \\ &= \frac{E}{V}\left[1 + (1+r)\nu g_{\mathcal{A}}(\nu)\right] \ , \end{aligned} \tag{3.6}$$

with the effective correlation function

$$g_{\mathcal{A}}(\nu) = \frac{(1+\mathcal{A}) - \nu\,(1-\mathcal{A}/8)}{2(1-\nu)^2} \ , \tag{3.7}$$

dependent on $\mathcal{A} = \langle a \rangle^2 / \langle a^2 \rangle$. Note that $\mathcal{A}$ is well defined for any size distribution function, so that Eq. (3.7) can also be applied to polydisperse situations. However, we remark that Eq. (3.7) is not appropriate for very wide size distribution functions [26], when higher order corrections have to be taken into account. Using the effective particle correlations, one can define the dimensionless pressure $P_2(\nu) = \frac{p^{\mathrm{m}} V}{E} - 1 = (1+r)\nu g_{\mathcal{A}}(\nu)$, and compare it with simulation results P. An almost perfect agreement between P and $P_2(\nu)$ is obtained for $\nu < 0.4$ and even up to larger $\nu \approx 0.65$, the difference is always less than about two percent. Note that the quality factors for *all* simulations collapse and that the quality is perfect (within less than 0.5 percent for all $\nu < 0.65$) if $P_2(\nu)$ is multiplied by the empirical function $1-\nu^4/10$, as fitted to the quality factor P/P_2. Thus, based on our simulation results, we propose the corrected, non-dimensional mixture pressure

$$P_4(\nu) = \frac{p^{\mathrm{m}} V}{E} - 1 = (1+r)\nu g_{\mathcal{A}}(\nu)\left[1 - a_g \nu^4\right] \ , \tag{3.8}$$

with the empirical constant $a_g \approx 0.1$, for all $\nu < 0.65$. Only in the monodisperse case, we use $P_4(\nu) = (1+r)\nu g_4(\nu)$, since this form is of higher order in the expansion around small ν and needs no empirical correction. For larger ν the excluded volume effect becomes more and more important, leading to a divergence of P. In the high density regime, the behavior is strongly dependent on the width of the size distribution function.

3.4. *A global equation of state (monodisperse)*

Based on both kinetic theory for the disordered regime and hard sphere simulations, a mixture pressure was proposed in a simple form, dependent only on the width of the size distribution $\mathcal{A}$. For higher densities and small width, $1-\mathcal{A}$, an ordered situation is obtained, whereas no order is evidenced for wide size distributions. The presence of an ordered situation is discussed below, in section 4. The dense situations, however, deviate from the prediction in Eq. (3.8) due to the excluded volume in a dense packing.

The equation of state in the dense phase can been computed by means of a free volume theory [6,27,28], which leads in 2D to the reduced pressure $P_{\rm sf} = 1/(\sqrt{\nu_{\rm max}/\nu}-1)$ [7], with the maximum volume fraction $\nu_{\rm max}$. Also slightly different functional forms $P_{\rm pm} = (\nu_{\rm max}+\nu)/(\nu_{\rm max}-\nu)-1$ [29], and $P_{\rm fv} = 2\nu_{\rm max}/(\nu_{\rm max}-\nu)$ [10], do not lead to much better agreement. Note that the above functions are identical, in leading order for small $\nu_{\rm max}-\nu$, so that we use $P_{\rm fv}$. Based on our numerical data, we propose the corrected high density pressure

$$P_{\rm dense} = \frac{2\nu_{\rm max}}{\nu_{\rm max}-\nu} h_3(\nu_{\rm max}-\nu) - 1 \ , \qquad (3.9)$$

where $h_3(x) = [1 + c_1 x + c_3 x^3]$ is a fit function with $c_1 = -0.04$ and $c_3 = 3.25$. To our knowledge, no theory exists, which combines the disordered and the ordered regime [8,9]. Therefore, we propose a global equation of state

$$Q = P_4 + m(\nu)[P_{\rm dense} - P_4] \ , \qquad (3.10)$$

with an empirical merging function $m(\nu) = [1 + \exp(-(\nu-\nu_c)/m_0)]^{-1}$ which selects P_4 for $\nu \ll \nu_c$ and $P_{\rm dense}$ for $\nu \gg \nu_c$ with the width of the transition m_0.

When the fit parameters $\nu_c = 0.701$ and $m_0 \approx 0.009$ are used, quantitative agreement between Q and the simulation results is achieved within about 1.5 percent (the agreement outside the transition region is much better than 0.2 percent). However, also a simpler version Q_0 without numerical corrections leads to reasonable agreement when $m_0 = 0.012$ and $\nu_c = 0.700$ is used. In the transition region, the function Q_0 has no negative slope but is continuous and differentiable, so that it allows for an easy and compact numerical integration of the pressure. We selected the parameters for Q_0 as a compromise between the quality of the fit on the one hand and the treatability of the function on the other hand.

The global equation of state can also be used for mixtures of particles with different sizes (data not shown here) if $\nu_{\rm max}$ is adjusted accordingly. For a more detailed comparison of the global equation of state with simulation data, see Refs. [7,10].

3.5. *Inhomogeneous systems*

Most of the data were obtained from elastic, homogeneous simulations. A few tests showed that also weakly inelastic situations lead to equivalent results as long as they are homogeneous. Data obtained from inhomogeneous systems which are not, in general, in global equilibrium due to *strong dissipation* can not be compared to the results presented. Work is in progress to check in how far subsystems in local equilibrium (or at least close to it) can be understood by the predictions valid for homogeneous, almost elastic systems. Note that the averaging in subsystems over short times introduces large statistical fluctuations, so that conclusions about one realization are not necessarily helpful. Furthermore, averaging is not possible over different realizations, since various local situations are incomparable from one run to the next and possibly even the global results differ.

4. How much disorder is necessary to avoid order ?

In order to study the deviation of the pressure p in the simulations from the theoretical value P_4 it is helpful to examine the quality factor $q = P/P_4$ more closely. In Fig. 1, q is displayed for various densities and dimensionless distribution widths of bidisperse systems with $n_1 = 0.744$ and $R \in [0.5; 1]$. In the contour plot (Left), q is plotted against the density, ν, and the width of the size distribution, $\sqrt{1-\mathcal{A}}$.

A valley in the q-surface corresponds to a reduction in pressure which we relate to order (which leads to a larger free path and thus to a reduced collision rate). The steep increase in the q-surface is due to the excluded volume of the particles. For every value of $\mathcal{A}$, one can obtain a specific value of the maximum packing density $\nu_{\max}$ by extrapolation.

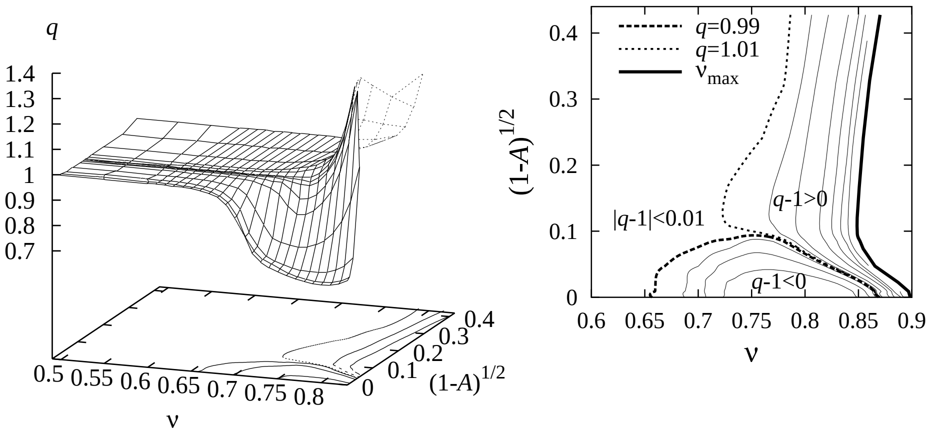

Fig. 1. Quality factor $q = P/P_4$, from simulations with different R- and ν-values, plotted against the volume fraction ν and $\sqrt{1-\mathcal{A}}$. The base of the left diagram and the right plot show the contourplot. Shown are the iso-lines for $q = 0.99$ (dashed), $q = 1.01$ (dotted), and $q = 0.75$, 0.85, 0.95, 1.05, 1.15, 1.5, 2, 3, and 5 (thin solid lines), as well as the maximum density (thick solid line). The maxima of the contour $q = 0.99$ is $\mathcal{A} = 1 - 0.093643^2 = 0.99123$, $\nu = 0.75199$, $R = 0.8143$

It can be evidenced that P deviates from P_4 by less than 1% at densities $\nu < 0.65$ regardless of the type and width of the size distribution function. For smaller $\mathcal{A}$-values, the prediction from kinetic theory is correct up to even larger densities. In the domain of agreement between theory and simulations, we assume that the system is in the disordered, fluid state. Consequently, the system is ordered, if a pressure drop occurs, i.e. if $q - 1 < -0.01$. The increase in pressure is related to the dense packing of the system and thus to the solid state, i.e. a solid has a much lower compressibility than a fluid. Note that the corresponding plots for other a polydisperse size distribution look very similar.

For broad enough size distributions, $\mathcal{A} < 0.99$, the disorder caused by the different particle sizes is sufficient to suppress the formation of an ordered structure. For our bidisperse systems with $n_1 = 0.744$, global disorder is predicted for $R < 0.814$. As a consequence, the pressure drop disappears and the validity of Eq. (3.8) is extended to densities up to $\nu \approx 0.75$ for very broad size distributions. For densities above $\nu \approx 0.75$ the pressure starts to increase strongly, exceeds the predicted value, and finally diverges when ν approaches $\nu_{\max}$.

The maximum packing density depends on the size distribution function and on the rate used to increase the density. Rapidly growing the particles increases the probability of trapping defects in the structure which results in a reduced $\nu_{\max}$. Here, we changed the density rather slowly, corresponding to the adiabatic limit, however, the rates of change are always finite in a numerical simulation.

5. Summary and outlook

A *global equation of state* for almost elastic 2D granular gases with mono-, bi-, and polydisperse size distributions was presented. For low and intermediate densities, the equation of state can be written in a closed form which only contains the width-correction $\mathcal{A} \le 1$ of the size-distribution function. A small, empirical correction can be added to the theories to raise the quality even further for medium densities. At high densities, the maximum packing density was obtained by extrapolation of the numerical data and a functional form was fitted to the high density, solid regime based on free volume arguments. Both the liquid and the solid regime were connected via an empirical merging function to give a *global equation of state* for *all* densities.

The simulations and the theories presented here were applied to homogeneous systems. The range of applicability may be reduced by the fact that dissipation can lead to strong inhomogeneities in density, temperature, and pressure. In a freely cooling system, for example, clustering leads to all densities between $\nu \approx 0$ and $\nu \approx \nu_{\max}$ [24, 30]. The proposed *global equation of state* is a necessary first step to account for such strong inhomogeneities with very high densities above which the low-density theory fails. Since the results are based on a limited amount of data, it has to be checked whether it still makes sense in the extreme cases of narrow $w(a)$, where crystallization effects are rather strong, and for extremely broad, possibly algebraic $w(a)$, where $\mathcal{A}$ is not defined. What also remains to be done is to find similar expressions not only for pressure and energy dissipation rate but also for viscosity and heat-conductivity and to extend the present results to three dimensions.

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References

[1] S. Chapman and T. G. Cowling. *The mathematical theory of nonuniform gases.* Cambridge University Press, London, 1960.

[2] J. M. Ziman. *Models of Disorder.* Cambridge University Press, Cambridge, 1979.

[3] J. P. Hansen and I. R. McDonald. *Theory of simple liquids.* Academic Press Limited, London, 1986.

[4] T. Pöschel and S. Luding, editors. *Granular Gases*, Berlin, 2001. Springer. Lecture Notes in Physics 564.

[5] L. D. Landau and E. M. Lifschitz. *Physikalische Kinetik.* Akademie Verlag Berlin, Berlin, 1986.

[6] J. G. Kirkwood, E. K. Maun, and B. J. Alder. Radial distribution functions and the equation of state of a fluid composed of rigid spherical molecules. *J. Chem. Phys.*, 18(8):1040–1047, 1950.

[7] S. Luding. Global equation of state of two-dimensional hard sphere systems. *Phys. Rev. E*, 63:042201, 2001.

[8] H. Löwen. Fun with hard spheres. In K. R. Mecke and D. Stoyan, editors, *Statistical Physics and Spatial Statistics*, Berlin, 2000. Springer.

[9] S. Sengupta, P. Nielaba, and K. Binder. Elastic moduli, dislocation core energy, and melting of hard disks in two dimensions. *Phys. Rev. E*, 61:6294, 2000.

[10] S. Luding and O. Strauß. The equation of state of polydisperse granular gases. In [4], pages 389–409; cond-mat/0103015.

[11] H. J. Herrmann, J.-P. Hovi, and S. Luding, editors. *Physics of dry granular media - NATO ASI Series E 350*, Dordrecht, 1998. Kluwer Academic Publishers.

[12] P. K. Haff. Grain flow as a fluid-mechanical phenomenon. *J. Fluid Mech.*, 134:401–430, 1983.

[13] J. T. Jenkins and M. W. Richman. Kinetic theory for plane flows of a dense gas of identical, rough, inelastic, circular disks. *Phys. of Fluids*, 28:3485–3494, 1985.

[14] J. J. Brey, J. W. Dufty, and A. Santos. Dissipative dynamics for hard spheres. *J. of Stat. Phys.*, 87(5/6):1051–1067, 1997.

[15] N. Sela and I. Goldhirsch. Hydrodynamic equations for rapid flows of smooth inelastic spheres, to burnett order. *J. Fluid Mech.*, 361:41–74, 1998.

[16] P. Sunthar and V. Kumaran. Temperature scaling in a dense vibrofluidized granular material. *Phys. Rev. E*, 60(5):1951–1956, 1999.

[17] J. T. Jenkins and F. Mancini. Balance laws and constitutive relations for plane flows of a dense, binary mixture of smooth, nearly elastic, circular discs. *J. Appl. Mech.*, 54:27–34, 1987.

[18] B. Ö. Arnarson and J. T. Willits. Thermal diffusion in binary mixtures of smooth, nearly elastic spheres with and without gravity. *Phys. Fluids*, 10:1324–1328, 1998.

[19] J. T. Willits and B. Ö. Arnarson. Kinetic theory of a binary mixture of nearly elastic disks. *Physics of Fluids*, 11(10):3116–3122, 1999.

[20] E. Dickinson. Molecular dynamics simulation of hard-disc mixtures. the equation of state. *Molecular Physics*, 33(5):1463–1478, 1977.

[21] S. Luding, O. Strauß, and S. McNamara. Segregation of polydisperse granular media in the presence of a temperature gradient. In T. Rosato, editor, *IUTAM Symposium on Segregation in Granular Flows*, pages 297–304, Dordrecht, 1999. Kluwer Academic Publishers.

[22] S. McNamara and S. Luding. A simple method to mix granular materials. In T. Rosato, editor, *IUTAM Symposium on Segregation in Granular Flows*, pages 305–310, Dordrecht, 1999. Kluwer Academic Publishers.

[23] B. D. Lubachevsky. How to simulate billards and similar systems. *J. of Comp. Phys.*,

94(2):255, 1991.

[24] S. Luding and S. McNamara. How to handle the inelastic collapse of a dissipative hard-sphere gas with the TC model. *Granular Matter*, 1(3):113–128, 1998. cond-mat/9810009.

[25] S. Luding, M. Huthmann, S. McNamara, and A. Zippelius. Homogeneous cooling of rough dissipative particles: Theory and simulations. *Phys. Rev. E*, 58:3416–3425, 1998.

[26] A. Santos, S. B. Yuste, and M. L. De Haro. Equation of state of a multicomponent d-dimensional hard sphere fluid. *Mol. Phys.*, 96:1–5, 1999.

[27] R. J. Buehler, Jr. R. H. Wentorf, J. O. Hirschfelder, and C. F. Curtiss. The free volume for rigid sphere molecules. *J. of Chem. Phys.*, 19(1):61–71, 1951.

[28] W. W. Wood. Note on the free volume equation of state for hard spheres. *J. Chem. Phys.*, 20:1334, 1952.

[29] E. L. Grossman, T. Zhou, and E. Ben-Naim. Towards granular hydrodynamics in two-dimensions. *Phys. Rev. E*, 55:4200, 1997.

[30] S. Luding and H. J. Herrmann. Cluster growth in freely cooling granular media. *Chaos*, 9(3):673–681, 1999.