Kinetic theory of a binary mixture of nearly elastic disks with size and mass disparity

Meheboob Alam[(1)], Jeffrey Willits[(2)], Birgir Ö. Arnarson[(3)] and Stefan Luding[(1,4)]

(1) Institut für Computeranwendungen 1,

Pfaffenwaldring 27, 70569 Stuttgart, Germany.

Email: alam@ica1.uni-stuttgart.de

(2) Computer Consultant, 3507 Lindell Blvd, St. Louis, Missouri 63103

Email: jeff@dcfc.net

(3) Kaupthing Bank, Armuli 13, 108 Reykjavik, ICELAND

Email: boa@kaupthing.net

(4) Particle Technology, DelftChemTech, TU-Delft,

Julianalaan 136, 2628 BL Delft, The Netherlands.

Email: lui@ica1.uni-stuttgart.de *or* s.luding@tnw.tudelft.nl

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Corrections are provided for two transport coefficients derived by Willits and Arnarson[1] for a binary mixture of nearly elastic, circular disks using the Revised Enskog Theory. The corrected viscosity coefficient is compared to the shear viscosity obtained from simulation results of a bidisperse mixture of inelastic, hard disks, undergoing uniform shear flow. The agreement is good for a wide range of sizes and masses.

I. INTRODUCTION

In a recent paper, Willits and Arnarson[1] (hereafter referred to as WA) outline a rheological model for a mixture of inelastic disks using the Revised Enskog Theory. Along with the balance laws for mass, momentum and granular energy, they derive the rheologocal equations of state for pressure, shear viscosity, bulk viscosity and thermal conductivity. To validate their arduous and extensive calculations they compare the results to molecular dynamics simulation of a binary mixture of elastic disks of almost equal mass and size. They show that their expression for the shear viscosity agrees excellently with the simulation results if equal or almost equal masses are assumed[6]. In our work, we show that WA's expression is correct only for the special case of a binary mixture with particles having equal mass, but significant deviations occur for the more general case of a mixture differing both in mass and size.

II. BACKGROUND

As a first step, we attempt to recover the known values for the monodisperse limit by assuming a vanishing fraction of particles of one species. Figure 1 shows the variation of the viscosity with the size ratio $R = d_l/d_s$ (d_l and d_s denote the diameters of larger and smaller species, respectively) for an equal-density mixture with a volume fraction ratio of $\nu_l/\nu_s = 10^{14}$, where $\nu = \nu_l + \nu_s = 0.3$ is the total volume fraction of disks. The solid and dashed lines represent the results of WA and the corrected expressions, respectively. Since the volume fraction of the smaller species is almost equal to zero, $\nu_s/\nu_l = 10^{-14}$, we expect the viscosity to be independent of the size-ratio; in contrast, however, the result of WA shows a monotonic decrease with R as observed in Fig. 1.

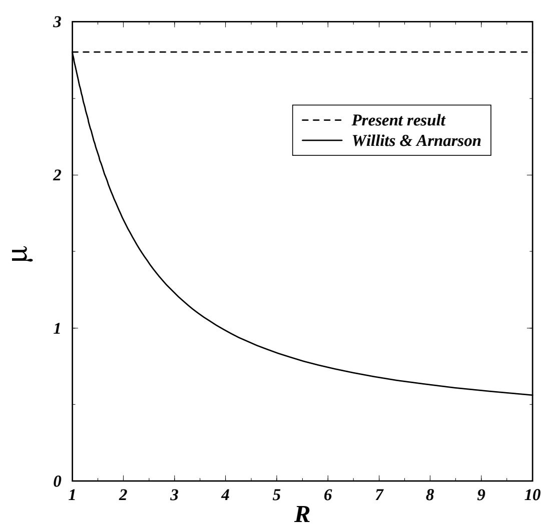

FIG. 1. Analytical results for the variation of the shear viscosity μ with the size-ratio R for uniform shear flow of an almost monodisperse mixture with volume fraction ratio $\nu_l/\nu_s = 10^{14}$ and the total volume fraction $\nu = 0.3$. The coefficient of restitution is $e = 0.99$ and the shear rate $\gamma = 1.0$. The viscosity has been nondimensionalised by $\rho_p d_l^2 \gamma$, with ρ_p being the material density of the particles. The solid line corresponds to the original results of WA, the dashed line denotes the results presented here.

Since the results did not agree, we derived the correct expression for the shear viscosity following the mathematical procedure of Ferziger and Kaper[3] and Lopez de Haro *et al.*[4]. Upon comparing our expression with that of WA, we found that a factor is missing from the coefficient of the Sonine polynomial expansion b_{i0} used in the expression for the shear viscosity. In the following, we briefly outline the procedure to obtain the shear viscosity of a binary mixture of hard disks.

III. SHEAR VISCOSITY

Let us consider a binary mixture of smooth inelastic disks of species l and s, with diameters d_i, masses m_i, and number densities n_i $(i = l, s)$. For the sake of an easy one-to-one comparison, we retain the notations of WA. The shear viscosity of such a mixture is given by[1,3,5]

$$\mu(N) = \frac{1}{2} T \sum_{i=l,s} \frac{n_i}{n} K_i' b_{iq}(N) + \frac{1}{32}\sqrt{\pi T} \sum_{i=l,s} \sum_{j=l,s} \left(2M_{ij}m_j\right)^{1/2} n_i n_j d_{ij}^3 g_{ij}, \tag{1}$$

where

$$K_i' = 1 + \frac{\pi}{8} \sum_{j=l,s} n_j M_{ji} d_{ij}^2 g_{ij}, \tag{2}$$

with $M_{ij} = m_i/(m_i + m_j)$, $d_{ij} = d_i + d_j$, g_{ij} is the contact value of the equilibrium pair distribution function, and T the granular temperature. $b_{iq}(N)$ in equation (1) are the coefficients of the Sonine polynomial expansion, with N being the number of Sonine polynomials used (i.e. N-th Enskog approximation). At the N-th level of approximation, the $b_{iq}(N)$ satisfy the relation

$$\sum_{q=0}^{N-1}\left[b_{iq}(N)\sum_{j=l,s} n_j g_{ij} B'^{ij}_{pq2} + \sum_{j=l,s} n_j g_{ij} B''^{ij}_{pq2} b_{jq}(N)\right] = 2nK'_i \delta_{p0}, \tag{3}$$

for all $p = 0, 1, ..., N-1$, and $i = l, s$, where δ_{p0} is the Kronecker delta, and B'^{ij}_{pq2} and B''^{ij}_{pq2} are the partial bracket integrals for hard disks[1,4].

We are interested in the first Enskog approximation ($N = 0$) for which we need to know the following two bracket integrals[1]:

$$B'^{ij}_{002} = d_{ij}\lambda_{ij}M_{ji}(1 + M_{ij}) \quad \text{and} \quad B''^{ij}_{002} = -d_{ij}\lambda_{ij}M_{ij}M_{ji}, \tag{4}$$

where λ_{ij} is defined by

$$\lambda_{ij} = \sqrt{\frac{2\pi T}{m_i M_{ji}}}. \tag{5}$$

At this level of approximation, equation (3) reduces to a set of two coupled algebraic equations for b_{i0}:

$$C_{ii}b_{i0} + C_{ik}b_{k0} = 2K'_i, \tag{6}$$

for $i = l, s$ and $i \neq k$, with

$$C_{ii} = \frac{n_i}{n} g_{ii} B''^{ii}_{002} + \sum_{j=l,s} \frac{n_j}{n} g_{ij} B'^{ij}_{002} \quad \text{and} \quad C_{ik} = \frac{n_k}{n} g_{ik} B''^{ik}_{002}. \tag{7}$$

The solution for b_{i0} is, for $i \neq k$, given by

$$b_{i0} = \frac{2(K'_i C_{kk} - K'_k C_{ik})}{(C_{ii}C_{kk} - C_{ik}C_{ki})}, \tag{8}$$

which, after some algebraic manipulation, simplifies to the expression:

$$b_{i0} \equiv \frac{2n}{n_i n_k d_{ik} g_{ik} \lambda_{ik}} \left[\frac{n_i K'_i \beta_i + n_k K'_k M_{ik} M_{ki}}{\beta_i \beta_k - M_{ik}^2 M_{ki}^2}\right], \tag{9}$$

with

$$\beta_i = M_{ik}(1 + M_{ki}) + \frac{1}{2}\frac{n_k}{n_i}\frac{d_{kk}}{d_{ki}}\frac{g_{kk}}{g_{ki}}\sqrt{\frac{M_{ik}}{M_{kk}}}. \tag{10}$$

Comparing with the expression for β_i given in WA on page 3119, we find that the second term in our expression for β_i has a factor $(M_{ik}/M_{kk})^{1/2}$ that is missing from the WA expression. The dashed line in Fig. 1 corresponds to the shear viscosity obtained using our corrected β_i from Eq. (10).

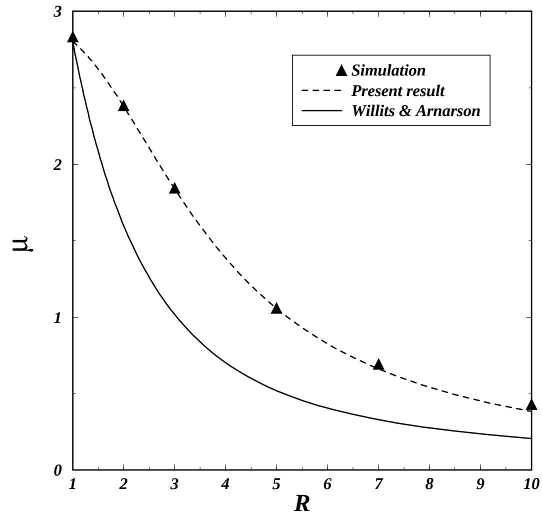

FIG. 2. Comparison of shear viscosity with ED simulations: $\nu_l/\nu_s = 19$; $\nu = 0.3$; $e = 0.99$; $\gamma = 1.0$.

In Fig. 2, we compare our expression for the shear viscosity with the simulation results of a bidisperse mixture of inelastic hard disks undergoing uniform shear flow; the simulation technique is the standard event-driven simulation. (The details of these calculations are the subject of a forthcoming publication.[2]) The parameter values are set to $\nu = 0.3$, $\nu_l/\nu_s = 19$; the coefficient of restitution, e, is 0.99 and the shear rate, γ, is 1.0. It is observed that the simulation results agree closely with the viscosity in Eq. (1) using b_{i0} from Eq. (9) with the corrected term in Eq. (10).

There remain quantitative discrepancies at large size ratios – for example, the theory underpredicts the simulation results by about 0.25% and 11% at $R = 5$ and 10, respectively. The result of WA underpredicts the viscosity levels significantly over the whole range of size-ratios for this set of parameters. It is worthwhile to comment on their comparison of the viscosity expression with the molecular dynamics simulation (see Fig. 1 in WA). The simulation results compare excellently with the analytical results since a binary mixture with particles having equal mass was considered. For this special case of equal mass, the missing factor in their expression for β_i is simply unity.

IV. HEAT CONDUCTIVITY

Without explicit derivation, we note that the term α_i on page 3119 of the paper by WA should be corrected[6] by the factor $(M_{ik}/M_{kk})^{1/2}$ as well, such that

$$\alpha_i = 12M_{ki}^2 + 4M_{ik}M_{ki} + 5M_{ik}^2 + \frac{n_k}{n_i}\frac{r_{kk}}{r_{ik}}\frac{g_{kk_c}}{g_{ik_c}}\frac{1}{M_{ik}}\left(\frac{M_{ik}}{M_{kk}}\right)^{1/2} , \tag{11}$$

with $k \neq i$.

Furthermore, the expression for the collisional contribution to the heat flux should read:

$$\boldsymbol{q}_{ij} = \frac{\pi}{2} g_{ij_c} r_{ij}^2 n_i n_j T \left\{ M_{ij}\boldsymbol{v}_i + M_{ji}\boldsymbol{v}_j - \frac{3M_{ij}M_{ji}}{2n}\left[(a_{i1}+a_{j1})\boldsymbol{\nabla}\ln T\right] + \frac{1}{n}(t_{i1}\boldsymbol{d}_i + t_{j1}\boldsymbol{d}_j)\right\}$$
$$-g_{ij_c} r_{ij}^3 n_i n_j T \left(\frac{2\pi m_i m_j T}{m_{ij}^3}\right)^{1/2} \boldsymbol{\nabla}\ln T \ . \tag{12}$$

It should be stated that a numerical check of the heat conduction properties of a granular mixture is not as straightforward as the test of the viscosity. While in the latter case the set-up of a homogeneous simulation is possible, the heat flux is only active in the presence of a temperature gradient, which typically involves also a density gradient. Those gradients however lead to segregation[7] and thus destroy the homogeneity of the system. For the additional problems occuring when a fixed density boundary condition has to be achieved see the study by Luding[7] and the references therein.

V. CONCLUSIONS

In summary, we have corrected the expressions for the shear viscosity and the heat conductivity of a binary mixture of hard disks in the paper by WA[1]. The resulting expression for the viscosity agrees well with the simulation results for a system of nearly elastic ($e = 0.99$) hard disks of equal density and different size, over a large range of particle size ratios. The corrected expressions for heat conductivity and collisional heat flux are only mentioned, but could not be checked in a similar, straightforward simulation.

Our work thus suggests that the first Enskog approximation for the shear viscosity is applicable to situations with extremely different particle sizes and masses[2], a promising perspective which should lead to further research in the field of granular mixtures.

VI. ACKNOWLEDGMENTS

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